The European Materials Modeling Council

The EMMC RoadMap 2018 for Materials Modelling and Informatics

For Europe, the EMMC – the European Materials Modelling Council – is proposing underpinning and enabling actions for the industrial implementation and exploitation of materials modelling and informatics, key building blocks to enhance industrial competitiveness and facilitate the digital transformation of industry. This RoadMap presents the needs of a broad and large community of stakeholders in the materials modelling and adjacent fields. The EMMC requests the EC to recognize the points identified in this Roadmap as being of Europe-wide interest. The proposed actions target TRL7 conform to the scope of the LEIT programme. The ultimate implementation (TRL 8-9) is up to the engaged material suppliers and end user product manufacturers as it can lead to proprietary knowledge with commercial potential. This phase however is not addressed in the 2018 RoadMap.

Disclaimer to the approach

The RoadMap recognises the importance of making advances in materials modelling to support the competitiveness of European industry. It strives to identify shortcomings and barriers in current approaches and proposes actions to address them based on rich input and discussions between the different stakeholder communities organised by the European Materials Modelling Council (EMMC). The stakeholders cover the whole spectrum of the materials modelling community in Europe:

- *Industrial users (manufacturers)*
- *Software owners*
- *Translators*
- *Modellers*

Often one organisation plays more than one of these roles.

The consultations across the broad spectrum of European stakeholders conducted by the EMMC proposes that the EU LEIT Work Programme 2021-2027 is used to further exploit the existing materials models and advance the successful transfer and implementation to industry. This equally fosters the capitalisation on the enormous knowledge potential through coordinating networks, integration of modelling into business processes, and easy access to modelling market places and validation facilities. The use of materials modelling is recommended for all LEIT activities as a means to reduce costly experiments, to use knowledge more effective and with greater agility use, and to transfer faster the technology within and across the participating industries and sectors. The RoadMap is a guide for the EU LEIT Work Programme towards a continued solidification and stimulation of industrial materials modelling in line with the fast-paced digitisation of society.

Summary

In 2018, the European Materials Modelling Council (EMMC) represents about 800 members with an interest in materials modelling. It promotes the application of materials modelling to support the European Industrial Competitiveness. The integration of materials modelling and informatics is considered future critical for more agile and sustainable product developments and use throughout the entire materials life cycle. It is aligned to the drive for a digital society that assists in developing a circular economy and addresses societal needs. To that purpose a materials modelling roadmap 2018 is proposed.

The vision is that by 2030, materials modelling is integrated as an operational discipline by the majority of European manufacturing companies to develop sustainable and competitive products taking advantage of an Open Innovation Platform providing source Quality Data, Translational Work Flows, and Software Algorithms available on an easy access federated grid.

It is the mission of the EMMC to make this possible by proposing a Materials Modelling Roadmap 2018 for Europe with topical actions that can be realised in the European Framework Programs. The document entails the state of the art in materials modelling, the challenges, knowledge gaps, and whitespaces, as well as actionable recommendations for projects. The ambition is to drive materials modelling towards at least a TRL 7 status and turning the vision into a reality.

The Materials Modelling Roadmap 2018 builds on previous roadmaps with a specific emphasis on stimulating continuity and a number of new topics. Each topic is an essential building block in a phased approach to accomplish the vision.

The key stakeholders are considered to significantly create added value and tangible benefits from materials modelling. For this to happen several critical challenges need addressing that are interlinked but can be treated as self-standing topical subjects.

- **Open Innovation Platform for Integration of models and modelling** for industrial impact
- **Facilitation of Translational Work Flow efforts** to match identified needs with materials modelling capabilities
- Creation of **Marketplaces and Data repositories** as part of the Open Innovation Platform to maximize materials modelling use for commercialising technologies fast
- Develop a **Materials Modelling Ontology** to provide a common materials modelling language that enable the relational integration of Translational Workflows
- Ensuring appropriate **Infrastructural Facilities and Interoperability** of materials models
- **Attract, educate and train** people for the use of materials modelling

The topical subjects form a logical sequence of complementing efforts. The Open Innovation Platform enables integration of models, which implies connecting in- and outputs to eventually address the industrial challenges. This requires facilitation i.e. making it easy for stakeholders to identify required models for use by following a Translation Workflow. The easily accessible one-stop marketplaces are then the virtual spaces that offer the models and accessories for use. A material's modelling ontology is required to make the identification and exchange possible through a common language expressing the relational context. All this happens in a digital space that necessitates infrastructural hardware but equally important inter-operational software accessories to make it possible. For this to happen competent people are needed at all levels for today and in the future.

Each of the topical subjects comprehensively considers: the state of the art, the EMMC ambition, and the EMMC approach, for how the implementation should take place for maximum success.

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1 Introduction

The RoadMap 2018 is elaborated by the European Materials Modelling Council (EMMC[1]). The EMMC has the goal to network existing and future activities happening in the field of materials modelling. The aim of the council is to establish current and forward looking complementary activities necessary to bring the field of materials modelling and materials informatics closer to the needs of industry (both small and large enterprises) in Europe.

How were the EMMC RoadMaps elaborated and endorsed?

In February 2014, 75 experts attended an EC Materials Modelling Policy meeting held at Covent Garden, Brussels. The views were captured in a Report "Materials Modelling: Where do we want to go" published on the LEIT website[2]. The EMMC was created with volunteers who started various working groups (WG) on materials modelling topics of general interest. Discussion notes were elaborated and an initial listing of 600 potential interested people and stakeholders was created and consulted to submit their interests and views. Subsequently and since then, the substantial comments and suggestions received have been captured into the RoadMap 2015. The extension of this RoadMap represented the Roadmap 2016[3], where more systematic inputs were collected by a dedicated online survey, which was sent to more than 1500 stakeholders.

In 2017, several EMMC workshops/expert meetings were organised (e.g. EMMC International Workshop 2017[4], EC/EMMC Translation Workshop[5], EMMC Workshop on Interoperability of Materials Modelling[6], EMMC Workshop on Model Quality, Gaps & Accuracy[7], EMMC Business Decision Support System Expert Meeting[8] etc.) with the goal to collect the opinion on different relevant topics from a number of stakeholders. The digested reports contributed to the latest updates and a view to the future in the current RoadMap 2018.

The EMMC continues to expand and its number of members - presently at around 800. The membership is free and aims to keep a close connection with the fast changing materials modelling capabilities and associated informatics tools. Consequently, the views expressed by the EMMC are generally endorsed by a significant number of stakeholders representing the views of a large and open materials modelling community.

[1] https://emmc.info
[2] "Materials Modelling: Where do we want to go?" Edited by Anne F. de Baas. http://ec.europa.eu/research/industrial_technologies/pdf/leit-materials-modelling-policy_en.pdf
[3] https://emmc.info/emmc-roadmap-2016/
[4] https://emmc.info/the-first-emmc-international-workshop-2017/
[5] https://emmc.info/events/translation-workshop/
[6] https://emmc.info/events/interoperability-in-materials-modelling-intop2017/
[7] https://emmc.info/emmc-materials-modelling-workshop/
[8] https://emmc.info/events/emmc-csa-bdss-experts-meeting/

2 Mission, Vision, and Objectives

The EMMC mission is to strive for the enhancement of the European Industrial Competitiveness through the integration of materials modelling and informatics enabling a more agile and sustainable development and use throughout the entire materials life cycle as aligned to societal needs.

Major trends that support this vision are as follows.

In recent years, materials modelling of nano-materials and systems has developed rapidly into software for practical use, in particular those based on discrete models (electronic /atomistic /mesoscopic). As a result, discrete modelling can be more widely used in industrial R&D and can be integrated with continuum modelling as evidenced by significant software industry acquisitions and mergers, for example the acquisition of Accelrys by Dassault Systems and the recent acquisition of QuantumWise by Synopsys. Importantly, there is a growing number of European SME's developing and marketing materials modelling software based on discrete models.

Still the European manufacturing industry continues to have a need for more capable, faster, more reliable materials models and related methodologies to sustainably produce and use materials in a multitude of applications critical to the functioning of society. It requires better modelling tools for validation and uncertainty quantification of materials performance, including linkable and coupled models. These allow closed loop optimisations by combining the simulation of manufacturing processes on all application-relevant materials and on all scales, component design and quality assurance. Additionally, better use of existing data as well as availability of more structured and validated materials information is essential for the ability to reliably simulate options and make sound data-based business decisions.

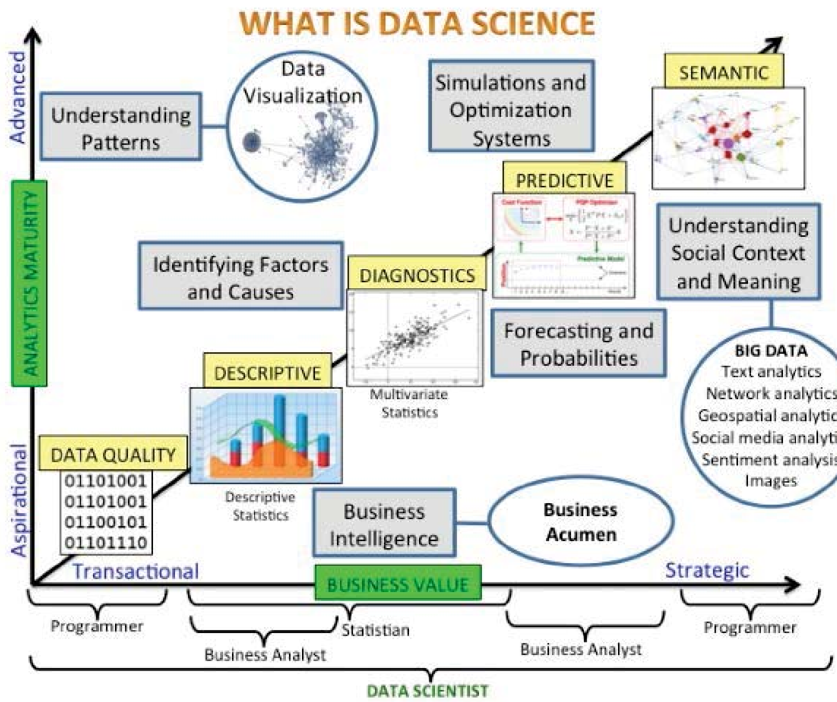

Figure 1 Data science with its maturity level

These requirements align very well with recent informatics advances in data science, machine learning and artificial intelligence. As shown in Figure 1, Data Science has been moving up the maturity and business value curve to the semantic level, enabled by the development of ontologies. Likewise, the data science about materials modelling, its classification and taxonomy and ontology has been taking significant strides, as evidenced by a recent CEN Workshop Agreement on materials modelling.

These developments make it possible to integrate a wide range of data sources. Advancements in machine learning and artificial intelligence methods (Figure 2) can then be brought to bear and drive the synergies between materials modelling and a wide range of soft data e.g. related to safety, life cycle assessment, regulations, consumer needs, and economic indicators.

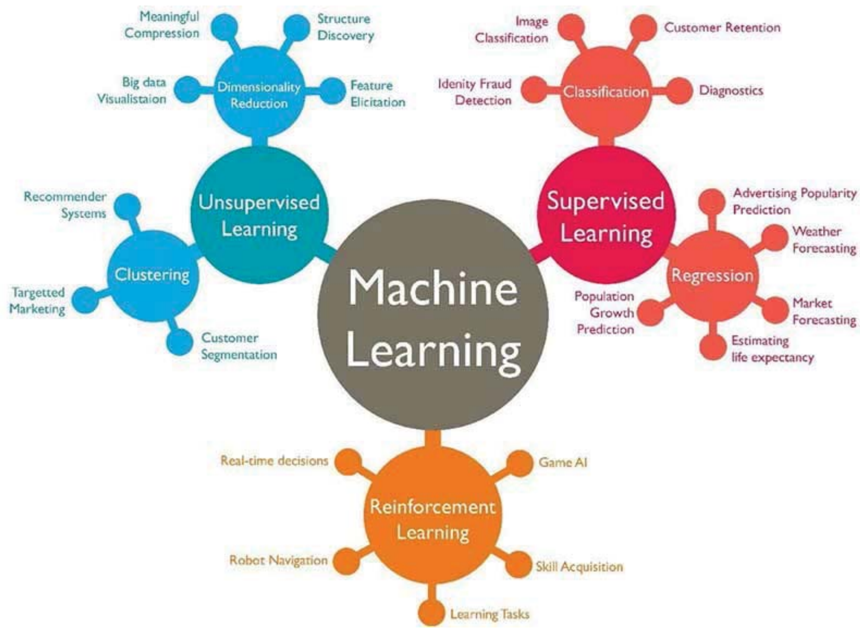

Figure 2 Advancements in machine learning and artificial intelligence methods

Accordingly, the objectives of the EMMC have evolved from the identified and critical core activities of having more capable, more accurate models, towards other essential materials modelling elements such as ontology development, information infrastructure, open simulation platforms, business decision support systems, open innovation platforms, quality databases and dataspaces, multiscale coupling science, education and translation activities, model qualification and validation in a Digital Materials Modelling Market Place.

The EMMC vision is thus shaped by considering all these elements together in a holistic fashion. Only then sufficient synergies can be created between all elements to address the most challenging questions in materials modelling today and in the future.

One central EMMC action is to enable manufacturers to utilise modelling in a much more integrated way in their materials and product development and business decisions. The ambition is to bring modelling one step closer to manufacturers towards a better integration into their various industrial processes. Along the way, there are many challenges, some of them are addressed in this road map, and many more will certainly be unravelled in the future. This RoadMap serves as a framework and is meant to be a strong basis to ignite further long-lasting activities within the materials modelling community and beyond in Europe.

3 Materials Modelling today

The development of new and improved materials and the use of existing materials in new applications across different industries are a significant innovation driver and a key factor for the success and sustainability of industry and European society in general.

Today, many more large and small companies rely on numerical simulations to effectively and efficiently design and engineer new products and to optimise processes, thus minimising the need for expensive and time consuming prototyping and testing. Furthermore, the **potential of materials modelling** as a driver for radical increase in speed of product design and radical decrease in production costs and in-service performance is recognised by manufacturing companies across Europe (SME's and large corporations alike). In a tough, highly volatile and competitive market environment, innovation and time-to-market is critical, especially for companies that need to put differentiated products on the market every year. Materials modelling-led product innovation can be a key differentiator for success in such competitive markets.

A key pillar in materials modelling is obviously the modelling itself. Here the quality of the modelling results and the speed with which they can be obtained are key factors in promoting the trust in and use of materials modelling in industry. Consequently, the identification of shortcomings in the available models and finding procedures to cure them are tasks of paramount importance to the EMMC and the entire materials modelling and industry communities. Examples of such shortcomings are the lack of adequate models (electronic, atomistic, mesoscopic or continuum) to simulate the complex problems predominant in industrial contexts; this has repeatedly been highlighted as a serious obstacle in the EMMC surveys. Thus, access to processes that enable to achieve needed model development including validation and verification – and in particular a work programme to carry it through – will open up a range of industrial applications to modelling. Validation of available and new models is crucial ingredients in this process but does not replace the need for new models where present ones are absent, failing or do not deliver the sufficient levels of validation enabling making business decisions on top of them.

While applications to both materials and manufacturing process design have been demonstrated, **modelling today is still and not always an essential component in a commercial or business development. Modelling tools are often seen as difficult to use**, **not accurate enough**, or unable to **get answers to very specific questions in a timely manner**. Equally important are considerations on the necessary investments in terms of people (expertise), infra-structure and capital in relation to the potential benefits in particular for smaller companies. Therefore, there remains a number **of technical challenges to develop predictive models and related tools that are easy in use and affordable yet accurate enough** to enable the desired novel product design and integration of business processes.

Numerical simulation in industry **today** is mostly dominated by continuum Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) models solved by Finite Element or Finite Volume Analysis. These continuum models form part of the Product Lifecycle Management/Computer Aided Engineering (PLM/CAE) process. This form of continuum- and system-based simulation of manufacturing processes, devices and products started more than 50 years ag an it comes as no surprise that it is considered as mature and is served by a limited number of multi-billion Euro software companies.

The influence of the material composition and structure on all hierarchical levels: electronic, atomistic, mesoscopic (including microstructure) on the macroscopic performance of the end-product is usually not taken into account in detail in such PLM/CAE methods. The continuum models for products and processes need to be linked to discrete models and applied to finer scales to give more insightful and accurate results. Recently, more companies have started using discrete (electronic/atomistic/ mesoscopic) materials modelling to include more detail in their simulations in order to design novel materials or do a better materials selection as aligned to the envisaged application and evermore stringent sustainability requirement. With the increasing importance of materials for the European competitiveness and sustainability, it is urgent today to further intensify the concerted actions of the entire **materials modelling community to mature models and related simulation tools for an effective and efficient use across various industry sectors and application areas facilitating their increased relevance and implementation for industrial exploitation**.

Typically, it takes 10 to 15 years to move academic software to marketable software. There is hence a need to produce more industry ready software by academic modellers and to stimulate the transfer of academic software to industry by sustainable business models. A common weakness in today's software lifetime is the discontinuity that takes place when the initial developers (e.g., Ph.D. students, post-docs) leave the development team, when public funding stops, the singular focus on the science and not on a supported, industrially viable software solution. Another issue in software exploitation is the software licensing scheme, which can be a bottleneck when transferring to or using academic software in industry, and is in many cases too restrictive. In fact, high-tech manufacturing industries have to rely on tools of highest quality, applicability, and long-term support. It is not the mission of academic research to provide these tools, but to work within an eco-system where academic creativity is professionally transformed and sustained. As TRL7 is the horizon of the present Roadmap, it needs to be understood that this document paves the way for the industrial deployment of materials modelling, but does not cover its use as mature, professional materials modelling software.

Moreover, much development in modelling and its application in industry are hindered by a lack of communication and interaction between different modelling communities that may have similar problems to address. This leads to severe waste of resources and limited use of models by manufacturers. The communication needs to be increased and other avenues to connect the stakeholders are required.

The gap in awareness, knowledge and skills and the lack of information about new developments and best practices are factors that hamper industry to unlock the potential benefit of current materials modelling technology fully. There is plenty of evidence that important and impact full topical challenges can be addressed with already existing materials modelling technology. Unfortunately, there is a lack of dissemination and translation of that knowledge into industrial applications. Equally important is the need for an open discussion forum on modelling approaches that do NOT work to constructively align efforts.

In manufacturing companies modelling typically resides within the realms of R&D and engineering departments while materials modelling is not yet used in daily operations. Here, materials modelling is still largely focussed on understanding of physical phenomena or figuring out why things do not work or could work. The importance of this should be used to make the next step towards integration of materials modelling into engineering design and business decision processes and systems to harvest its full benefits.

While there are many success cases of scientists in manufacturing industry (often supported by scientists at software companies) translating business problems into problems that can be solved by materials modelling, the vast majority industrial scientists neither have the resources nor the skills to do so. **Manufacturing users of modelling, in particular SMEs, quite often have a lack of expertise that prevents them from integrating materials modelling into their development and production workflows reliably**. There is hence **a need for players** who have the ability **to translate industrial problems into cases to be simulated.**

Another factor currently resulting in a **lack of acceptance** of materials models and model systems is a **lack of validation**. Furthermore, in conservative fields such as aerospace and health, lengthy certification processes are required entailing significant investments. In other words, acceptance and adoption of modelling materials properties instead of experimentally measuring them for certification and validation purposes can and must be enhanced.

There is therefore a need to establish a trusted process that incorporates more models into the materials design and manufacturing processes.

Numerous modern numerical methods and software packages have been developed both by academic and industrial parties that allow fast and reliable simulations of many materials properties and systems for a large variety of technological processes. The number of key players and stakeholders engaged in the various modelling activities, including electronic, atomistic, mesoscopic and continuum models (e/a/m/c) in Europe is rather huge. The explosion of the number of models (of mostly the materials relations, and the data related to these models) makes it **difficult to find the most relevant solutions in a timely manner** and it is often unclear which models and which software tools are available for a particular physics/chemistry or technical problem. *There is currently no common platform that manages the materials data and knowledge infrastructure simultaneously.* In addition, even when specific models are available they often don't fulfil the needs of modelling and simulation of interrelated engineered systems in an industrial context involving complex decision-making processes[9]. It is very hard to link and couple them for closed loop optimisations. For example, in manufacturing processes where material properties are defined, components are designed, and quality assurance and evolution of properties must be conducted during service.

Therefore, there is a need for improved linking and coupling of models to describe all relevant phenomena. One also needs to consider the interoperability between materials models and between experimental and numerical simulations and how they can be integrated. This presents an added value to the workflow of material design and is poised to increase the reliability of modelling. **In order to achieve this, the current lack of interoperability and standards should be alleviated**. Linking requires transferring of data and knowledge from one scale and model to another and demands an **efficient management of data**, including publishing, validating, linking, archiving and retrieving of (virtual) modelling data and knowledge in a well-structured and standard form.

[9] C. J. Kuehmann and G. B. Olson, "Computational materials design and engineering," Materials Science and Technology, vol. 25, no. 4, pp. 472-478, Apr. 2009.

There are substantial barriers in the way to integrating materials models and databases into business decision support systems. Materials models often lack the required level of accuracy, robustness and uncertainty (technical and financial risk) quantification for the specific design, as well as speed to allow a large design space to be explored. Models also need to be highly cooperative to determine the best combinations of process and composition to meet a diverse set of material objectives. It often requires a multi objective optimisation procedure that goes beyond and is in addition required to the specific materials models used.

Successfully addressing all these challenges allows reducing the time to market and development costs of differentiated product offerings leading to major benefits and enhanced competitiveness for the European industry base as a whole in a global economy.

4 Stakeholders

When considering the activity of materials modelling in all its aspects several stakeholders can be identified. In essence, a circular value chain can be identified from academic knowledge workers to industrial users of modelling, here referred to as Manufacturers, who define the needs as driven by their commercial interests. The technical part then stimulates modellers to develop the potential tools that can address these challenges. Accordingly, four classes of stakeholders can be defined: Manufacturers (both material suppliers and product manufacturers), Translators, Software Owners, Modellers. The EMMC represents the interests of all stakeholders.

4.1 Manufacturers (MAN)

The group of Manufacturers represents the interests of (current and future) users of materials modelling and product developers - small and large companies of the European manufacturing industry. It gathers key company representatives across industrial sectors, from consumer goods to industrial chemicals, from chemicals and polymers to metal and ceramic alloys, covering aspects of feedstock to product applications and their cradle to grave life cycle. The interest of this stakeholder group is to clearly articulate commercial user needs when introducing materials modelling into their business cycle. The EMMC takes action to identify key areas of company interest for materials modelling solutions, and how those solutions can be achieved, while the group acts as a sounding board and participates in European consultation initiatives.

4.2 Translators (TRANS)

The successful integration and application of materials modelling in industry depends heavily on translating industrial problems back into scientific questions that can be addressed with (existing) modelling software, i.e. typically performing a process of understanding well the business case and the industrial technical challenge and correlating it to the most suitable modelling tools used by the most suitable modelling executors. In fact, no industrial project using materials modelling could ever be launched without some translation effort. Typically, the 'Translator function' is performed by different actors, including R&D staff in large enterprises, application scientists in software companies, scientists and engineers in research or knowledge institutions as well as individual consultants as experts in the field. While the role as such already exists to some extent, there is however no wide-spread recognition of the Translator as a key actor having a well-defined role. Establishing Translators as recognised actors requires the creation of a set of open and transparent conditions and best practices demonstrating the translation process for different types of industry and establishing a database of competent Translators, available to industry, in particular to SMEs.

The group of Translators within the EMMC consists of people, experienced in "translation" and encompass representatives from industry, knowledge institutes/universities, SWOs and independent Translators/consultants. Although Translators have a working knowledge of how to approach industrial challenges by materials modelling and their role is well defined, there is a need to further broaden the description of the Translators. Specifically, to consider estimation of technical quality attributes of modelling (Key Performance Indicators KPI), and business-related measures like pricing, return on investment, time to market, and sometimes even regulatory and legislative issues. This aspect of "translation" is usually not yet taken into account and can be a reason why industry is currently not fully unlocking the potentials of modelling. Translators within the EMMC need to take these business-oriented measures into account from the very beginning to the benefit of manufacturers.

The Translator's role is not meant to replace or overlap with existing translation efforts, but rather to clarify, set standards and significantly extend or enhance their functioning through a more complete and wider expertise offering. The EMMC will offer a database of Translators and will facilitate the needed broadening of Translators' expertise to more efficiently implement the use of materials modelling in industry.

4.3 Software Owners (SWO)

Software owners are those stakeholders (academic or commercial) who actively make their software available to third parties by a wide range of licensing schemes. This stakeholder group includes academic software owners who offer their software with or without charge as open source code, and commercial software owners who sell or licence their software as sustainable business. A key driver of commercial software owners is the creation of industrial value for the end users, in particular in the manufacturing industry, but also for academic users, while software owners from academic institutions also benefit from recognition in their community, e.g. by citation of their work.

The Software Owners group helps articulating policies and programmes supporting academic and commercial software owners and it identifies modelling gaps. The group has already established guidance on quality assurance in software development to support the process of transferring academic software to the manufacturing industry. This document can be found on https://emmc.info. Licensing policies, standards and software documentation are discussed and recommendations are made.

4.4 Modellers (MOD)

The Modellers stakeholder group consists of the developers and users of materials models and modelling, located in industrial, academic and a range of other settings. More specifically, the MOD group may be developers of theory, mathematical concepts, algorithms, respective solvers, coupling and linking schemes and computational codes for electronic, atomistic, mesoscopic and continuum models to study the material properties and behaviour. Depending on the occasion, the MOD stakeholders can be meaningfully classified according to a range of schemes representing their expertise or primary activities, for example expertise in various technical aspects of modelling and simulation (MD expert, continuum modeller, ...), type of materials expertise (soft-matter, semiconductors, hard materials, ...) or application domain and phenomena (electrochemistry, magnetism, catalysis, ...), and so on.

The scope of the MOD stakeholder group within the EMMC encompasses two main efforts: on the one hand, the stimulation and wider exploitation of existing models, and on the other, the analysis of the state of the art and establishment of a RoadMap for further research necessary for the development of new or improved, more accurate, reliable (yet computationally feasible) models of industrial relevance.

4.5 European Materials Modelling Council: Stakeholder organisation

There is and will be a need for an overarching organisation that build-up the materials modelling constituency and networks the relevant stakeholders. There is a need for increased interaction between the multitude of stakeholders and a common representation to stimulate exploitation of materials modelling. The EMMC is established to fulfil that role and as such can articulate the needs and equally advertise the benefits of materials modelling. These elements form the base for RoadMaps that formulate and can guide the necessary actions to be taken for achieving the vision.

5 Industrial Integration and Economic Impact

5.1 State of the art at present

With the increasing importance of materials as limited or renewable feedstock for the European industry in terms of its global competitiveness and long term sustainability, there is an urgent need to continue and maintain the fostering and **development of a materials modelling community. This community captures the present and future materials knowledge in a digitised format for the effective and efficient use across various industry sectors and application areas**.

Furthermore, the **potential of materials modelling** as a driver for the radical **increase** in speed of product design and the radical **decrease** in manufacturing cost and in-use performance is recognised by manufacturing companies across Europe (SME's and large corporations alike). In a tough, highly volatile and competitive market environment, innovation and speed-to-market is critical, especially for companies that need to put differentiated products on the market every year. Materials modelling-led product innovation can be a key differentiator for success in such competitive markets.

Today, many large and small companies alike rely on numerical simulations to effectively and efficiently design and engineer new products in order to minimise the need for expensive and time-consuming prototyping and testing.

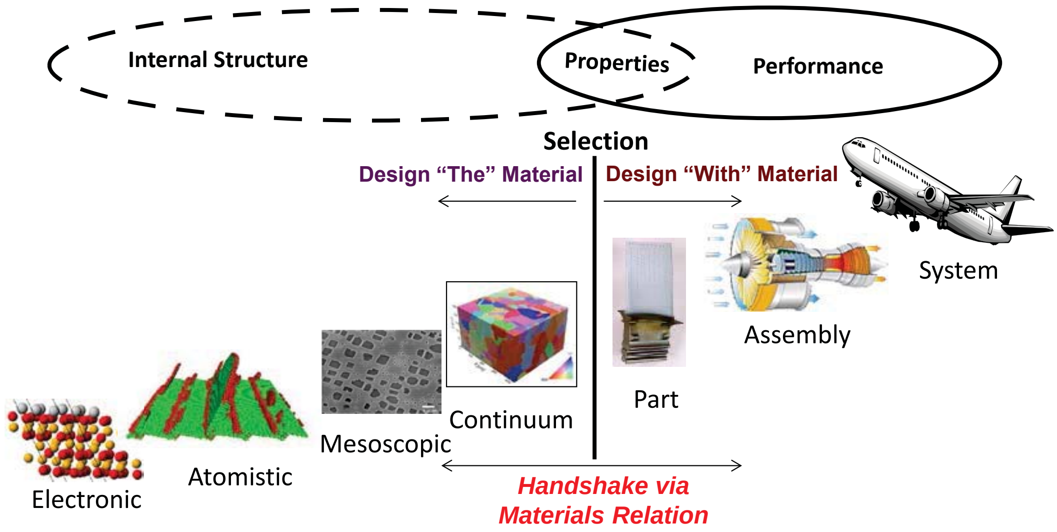

Figure 3 Stages of materials and product design[10]

Numerical simulation in industry today is widely used in the 'Design "WITH" material' phase of development as shown in Figure 3. It is mostly dominated by continuum modelling, which is part of Computer Aided Engineering and Design (CAE/CAD) and Product Lifecycle Management (PLM). This simulation of manufacturing processes, devices and products started more than 50 years ago, is mature and served by a limited number of multi-billion dollars software companies. The influence of the chemical material composition and structure on the macroscopic performance of the end-product is usually not taken into account in detail in such PLM/CAE methods. Product development with these methods basically assumes the material as fixed and characterised to have certain material functional properties.

The need to improve the accuracy during product design, the increased reliance on micro- and nanoscale materials features to drive improvements in product properties, alternative materials and renewability or recycling requirements has been and is driving the need to apply materials modelling at finer scales even in the 'Design with materials' stage. This has meant that more and more companies have started using continuum models applied at the micro-structural scale as well as discrete materials models linked to continuum models. Evidence for that is also seen in related software mergers and acquisitions (e.g. e-Xstream-MSC Software, QuantumWise-Synopsys).

Considering the 'Design "THE" material' phase of development (as shown in Figure 3) materials modelling has been used in industrial R&D for about 30 years. It has been adopted as an R&D 'tool' in the chemicals, electronics, energy, materials, pharmaceuticals, and personal care sectors by all large and a number of medium as well as some small companies. Its impact on efficiency and effectiveness of R&D as well as value-chain interactions (between suppliers and manufacturers), communication and marketing have been well documented in success stories and impact reports.

The increasing industrial integration and impact can also be measured by the steady growth of the related software sector, the number of trained professionals active in the field, and the growth in the amount of computing (including High Performance Computing) applied in this sector. A recent example

[10] David Cebon, Granta Design, Presentation at EMMC International Workshop2017, Vienna, 5-7 April 2017

is the supercomputer that was put into operation at BASF in October 2017 (ranking in the top 100 in the world), which to a significant part is dedicated to their chemicals and materials modelling effort.

However, in the ‘design “THE” material’ stage, materials modelling typically resides purely within the realms of R&D departments concerned with long term projects focussed on understanding of physical phenomena rather than for use in daily operations and business decisions. While the importance of the former should not be diminished, it is not sufficient for integration into engineering design and business decision processes and systems.

Also, **modelling today is not always the essential tool in commercial materials development** because **modelling tools are often seen as difficult to use**, **not accurate enough**, or unable to **get answers to very specific questions in a timely manner**. There remain a number **of scientific and technical challenges to develop predictive models that are easy in use and affordable yet accurate enough** to enable the desired novel product design. There are also still organisational and language barriers that hinder the successful integration of materials modelling in an R&D process, and in some cases even successful materials modelling efforts have been disbanded as a result of organisational changes, as modelling is often regarded as a cost rather than a “digital asset”.

The gap in awareness, knowledge and skills and the lack of information about new developments and best practices are factors that hamper industry to unlock the potential benefit of current materials modelling technology fully. There is plenty of evidence that important and impact full topics can be addressed with already existing materials modelling technology. However, there is a lack of dissemination and translation of that knowledge into industrial applications, as well as a lack of public discussion about approaches, which do NOT work.

Recently, digitalisation, the advent of ‘big data’ and related analytics is starting to influence the way in which materials modelling is regarded as part of the R&D enterprise. Related digitalisation is also the trend that materials companies are starting to supplement their products with materials models in their offering to customers (so-called product+ or a product’s digital component) to differentiate themselves from competition.

Hence, in summary, the status is that

- The potential of materials modelling as a driver for more efficient and effective product innovation is recognised by manufacturing companies across Europe.
- A large part of materials modelling investment and use relates to continuum modelling during the “Design WITH material” stage of product development.
- Microstructural continuum modelling and discrete modelling is growing strongly in use in the “Design WITH material” stage due to ever increasing demands on product features and properties.
- Materials modelling in the “Design THE material” stage has experienced slow but steady growth in the last 30 years. Success and industrial impacts are clearly demonstrated. However, more sustained adoption is still hampered by a number of factors including time scale, system complexity, controlled accuracy, usability, lack of integration.

- Recent developments in digitalisation and big data are likely to influence the way in which materials modelling is regarded as a potential digital asset that captures in house knowledge and allows easy access of distributed datasets.

5.2 EMMC Ambition

With the advent of big data, data driven materials modelling is playing an ever-increasing role. It is important to note that in industry, it is not about theory driven versus data driven materials models. It is about finding a solution to a problem, and the cost and speed at which that is done. How that solution is found has no or is of lesser importance. Whereas theory driven models can help to develop a more fundamental understanding and to extrapolate in unknown areas, data driven models can help to bring accuracy in areas where “real life” systems deviate significantly from “model or ideal” systems, to bridge gaps in fundamental understanding, or act as a meta-model or emulator for time-consuming theory driven models. So-called hybrid approaches where theory driven and data driven materials modelling are being combined will become more and more important.

There is an opportunity for materials modelling to be developed further to become a valuable source of data in the ‘big data’ realm. As such, materials modelling will become an integral part of a digital R&D organisation. It will support new value chain interactions and business models emerging in the fourth industrial revolution.

The development of standards, metadata and ontologies will enable materials modelling and materials characterisation to become more strongly intertwined. Together they (and the data and knowledge they provide) will become part of a range of digital assets that drive more efficient and effective development of new and advanced materials as well as products designed with these materials. Digitalisation in combination with physics and data-based materials modelling will furthermore help to overcome the current divide between “Design THE Material” and “Design WITH Material” phases, creating a digital continuum from the chemistry to the consumer and back. It will support companies to respond to societal challenges of the 21st century and deliver more customer responsive and personalised products as the ability to cross the design divides diminishes.

As a result, materials modelling will become more naturally integrated into business decisions. A Business Decision Support Systems (BDSS) is about combining materials models with other sources of information, and turning it to actionable knowledge that drives business decisions based on selected key performance indicators (KPIs). Due to the level of complexity multi-scale materials models might be challenging at times to be embedded in a BDSS, whereas data driven materials models are somewhat more accommodating. Irrespective, an additional level of algorithms will be needed for handling the multi-objective functions and thus directly linking materials modelling with advanced data analytics methodologies i.e. informatics (self-learning, neural nets, genetic algorithms, block chains, Pareto fronts).

There will be systems that chose the level of materials modelling sophistication required for a particular purpose that it is used for. More, relatively unsophisticated materials models will be applied by users from technical service and development, customer support and marketing, but these models will sit in a digital continuum connected to validation data and more sophisticated models. Key will be the ease for them to use these models as well as their relevance to the questions they are trying to answer.

In some cases, a qualitative answer from a materials model is sufficient for obtaining a trend or relative comparison (e.g., predict properties of different materials to be tested to allow for a smaller experimental design), in other cases, a quantitative answer is required to make an absolute decision or obtain an accurate input for further calculations (e.g., decide if the material of choice will sustain an impact).

Furthermore, materials models will enable companies to supplement their products in their offering to customers (so-called product+ or a product's digital component) to differentiate themselves from competition. Moreover, materials models can become much more than an R&D tool, but a means of capturing materials design and behaviour such that it can be re-called not only by end users of the material (e.g. plastics manufacturers) but throughout the materials life cycle, for example supporting future damage repair and end of life decisions.

5.3 EMMC Approach

In order to widen the success of materials modelling throughout European industry, including SMEs, actions to overcome some of the barriers are needed that might differ and need to be tailored depending on the particular stakeholder.

In order to better integrate materials modelling into industrial processes and bring modelling on the critical path of commercial product development, materials modelling needs to be integrated into the high-level trends in industry, including digitalisation (including digital twin and V+R developments), Industry 4.0, including new business models based integration of models and products (Product + etc.). Materials Modelling needs to be more tightly integrated into these emerging informatics systems, become a de facto data source on a par with a range of other data sources. Furthermore, materials modelling needs to be set up to contribute to delivering on the promises of Artificial Intelligence application in R&D. There are already a number of promising examples of increasing the efficiency and effectiveness of materials and product development by means of joining materials modelling (data and physics based), experiment/characterisation and machine learning. Utilising and integrating with these developments will further boost the utilisation of materials modelling in business decisions.

Integration of materials models in product life cycle management requires a joint-up information framework. Ontology developments in the PLM, materials and materials modelling areas should be interlinked in order to enable all stakeholders to build systems and communicate on a shared semantic basis.

However, it behoves an organisation such as the EMMC to warn about the dangers of "overselling" and hype, which can cause long-lasting damage to the field. Discrete materials modelling technology has to be built on the best scientific capabilities, advanced mathematic algorithms, and implemented with the highest standards and practices of software engineering while clearly recognising the boundaries of accuracy and predictive power. It is obvious that meeting these challenges requires intellectual efforts and investments which can adequately only be achieved by a creative process connecting academic research with professional software development and deployment.

6 Industrial Software Deployment

6.1 State of the art today

Compared with North America, Japan, and Korea, the European manufacturing industry has been late in adopting materials modelling on the discrete level. For example, General Motors in the USA and Toyota in Japan have been practicing advanced materials modelling on the electronic-structure level since over two decades, European car manufacturers have built materials modelling groups with capabilities in discrete modelling only in the last few years. Smaller European companies and SME's are still far from benefitting directly from today's capabilities of discrete materials modelling. This situation is a paradox as the leading electronic structure programs for materials modelling have been developed in Europe. For example, the Vienna Ab initio Simulation Package (VASP) is undoubtedly the most respected and used computer program of its kind, yet the industrial benefits have been mostly reaped by non-European companies. In the case of VASP, at least there is an economic return in the form of license fees flowing back to the original developers of the program, thus securing a stable financing of code developments. The situation is even more grotesque with free open source codes such as Quantum Espresso, where non-European industries use the fruits of European creativity without any direct economic return to the European tax payer. Fortunately, this situation is currently changing, and more European companies are asking for materials modelling software. Furthermore, there is a growing awareness that advanced and integrated software for materials modelling represents an opportunity for a budding new software industry. In fact, Europe has the opportunity to become a world-wide leader in this new industry sector of the 21st century, provided that wise and forward-looking decisions are taken.

From many discussions with the various stakeholders and the focussed actions, surveys and expert workshops of the EMMC it has become evident, that the main reasons for the hesitant uptake of discrete materials modelling by the European industry include:

- Shortcomings of current simulation technology to handle complex system
- Lack of accuracy of current models
- Short-term focus of industrial technology management
- Perception that modelling especially on the electronic/atomistic/mesoscopic levels is more of an academic research activity than an industrial necessity

It has to be said that leading European companies such as BASF and Shell have a long tradition of materials modelling, for example in the areas of catalysis and in polymer science with well-established and highly competent teams. However, overall, the use of discrete materials modelling in the European industry is still rudimentary.

The perception that discrete materials modelling does not provide enough economic value for the European industry because of intrinsic shortcomings to handle complex systems with sufficient accuracy is in part cultural roots. Japanese companies, for example, tend to think more long term and are willing to invest in activities with returns in 10 to 20 years. Another factor is the need of European industrial R&D centres for extremely powerful and accurate modelling capabilities, since their products and processes are highly sophisticated and complex. Thus, it is very hard to provide a value added through modelling and simulations. Academic software usually is not intended and falls short in meeting such stringent requirements.

Another practice of European industrial organisations is the outsourcing of up-stream and exploratory research to universities. Materials modelling falls often into this category. The return is often as one can expect, namely good academic research and publications after years of efforts. The result is a self-fulfilling prophesy: materials modelling does not have industrial maturity. Free, open source software aggravates this perception.

6.2 EMMC Ambition

The European industry should have the highest quality materials modelling software, professionally supported and seamlessly integrated in their R&D workflows. Professional software has to be rich in capabilities, reliable, validated, supported, and it has to focus on productivity, i.e. ease-of-use. The time of researchers and engineers in the European high-tech industry is extremely precious.

A key purpose of the LEIT programme is to raise the economic agility of European industry by transferring and stimulating the use of materials modelling software and methodologies, initially developed often in academic groups, into the industrial practice. It has been recognised that there is a need to lower the entry barriers by producing better structured and tailored software. This holds in general for the code, data standards and integration of codes. However, the direct use of academic software by industry leads at best to TRL7. Experience in our industrialised society shows that the subsequent wide-spread deployment of such innovative technology is best done by industrialising also its deployment. For example, this was the case x-ray spectrometers, which nobody in industry or even in universities would contemplate to obtain in any other way as from industrial suppliers who have perfectionated this technology. Fundamentally, advanced materials modelling software is not different.

Three phases in software development can be distinguished:

PHASE I: Exploratory phase (new functionality of models)

> In this phase, new models are explored with innovative concepts from physics, chemistry, and applied mathematics. The development is predominantly science-oriented and the models are applied to a few specific test cases. Exploratory model development takes place mostly in academia. Software developed at this stage has rapid-prototype character, *i.e.* it is not designed to be user-friendly and is often shared freely among scientific colleagues. IP protection is usually covered by the academic code of conduct only. The question of legal ownership (not to be confused with authorship) of the software is often considered secondary at this stage. Important ideas and algorithms are usually published in the scientific literature in refereed journals.

PHASE II: New materials modelling software

> In this phase, new materials modelling software has been validated on a set of test cases. It has thus proven wider applicability and it has the potential to solve new problems of value to industry. While in the early stages of this phase the software is still in a prototype phase, the use of the software by a wider, still mostly academic community and application to a wider range of systems contribute to further maturation of this software leading to improved robustness, application of software engineering principles, and documentation.

PHASE III: Commercial modelling software

> This phase is concerned with the commercial scale-up of software for more than a small community of end-users. Commercial software companies provide integration in comprehensive software platforms, systematic verification, full validation, documentation, user-friendly interface, testing suites, durability. Long-term support systems are developed since the life span of successful commercial software extends over many decades. Successful materials modelling software companies require team members of the highest scientific quality and experience ("domain experts") working closely together with industrial customers on the one hand and with internal experienced software engineers ("core developers") on the other hand.

The target of EU-LEIT research and innovation funding will be to reach at least Phase II in their projects since it will help to bridge the gap over the software "valley of death". Guidance should be elaborated to ensure that academically developed software will be more easily picked up by Software Owners who take the development to Phase III. This will often happen in close collaboration with the original software developers if they wish to be part of the exploitation phase or in collaboration with Translators who use the code themselves in industrial research.

In order to decrease the weakness related to the discontinuity that usually occurs when the initial developers are no longer active or leave the development team, or when the software is transferred from academia to commercial software developers, the software quality needs to be guarded from the early stage onwards. Use of data standards may also substantially contribute to ease of maintainability and sustainability of the software, lowering also the efforts needed to get to Phase III. Quality assurance on models and software should be implemented throughout the **academic and commercial** development process.

Quality is described in two ways:

- Ability of the model to solve the initially defined problem:
    - Is the solution accurate?
    - Is the solution precise (enough)?
    - Is the solution easy/possible to implement into an industrial framework?
- Software quality is a.o. determined by:
    - Generality, stability and resilience
    - Performance (CPU and memory requirements, etc.)
    - Maintainability and extensibility
    - Compliance with standards
    - Interoperability

If software possesses these qualities, this means that software is easy to maintain, understand, improve and adapt by any developers (not only the original creators).
In order for academically developed software to be employed by industry the software in Phase II should be developed based on the following quality recommendations[11]:

[11] See, for example, Christensen *et al*., Integr. Mater. Manuf. Innov. **6**, 92 (2017)

- proven wider applicability via validation on a set of fully documented test cases
- documented results obtained in collaboration with industrial users solving specific industrial problems
- documented accuracy/functionality proven in high profile academic publications (especially important in some markets,
- good numerical implementation, proven numerical stability (using test suites)
- good documentation of underlying equations and algorithms, validation cases, boundaries of validity, clear mapping of raw formula to code variables
- clear documentation of which version of the code was used to obtain what result and content of the next upgrades (not necessarily professional version control, though it is preferable)
- licence allowing commercial industrial use and exploitation, but still allowing academic modellers to enjoy the fruits of their work in the future, e.g., by partnering with commercial distributors.

Software engineering courses are recommended at the onset of the development process as there is a need to improve skills of academic modellers (physicists and chemists). This can be addressed by strengthening the link between academic developers and industrial development teams. Commercial software owners who base a substantial portion of their portfolio on academic software have a genuine interest in supporting the development of such software and seek active participation in EU projects alongside the academics to ensure an early adoption of good software engineering practises. They could function as mentors of the PhD students. Proposals should demonstrate a confidence inspiring approach to guarding software quality. More widely, this could be done by having a supported programme for internships of PhD students in software development companies.

Licensing schemes should be used that do not block commercial exploitation. Regarding licensing of software, it is of utmost importance that academic software developers receive better information on alternative licensing models that do not preclude commercial exploitation while protecting the original academic developer rights.

6.3 EMMC Approach

Nothing succeeds like success! With this guideline in mind, the path to industrially valuable materials modelling software should involve all players in success-oriented missions, namely scientists and engineers from the manufacturing industry, theoretical, computational, and experimental scientists and engineers from commercial software companies in cooperation with academic and research organisations as well as experts in data science. Building on the data and knowledge gained in the activities of the EMMC and its network, the following steps will lead to success:

- Clear definition of the industrial goals and needs. This involves the articulation of the envisioned industrial products, for example in the domains of energy, e-mobility, health and environment and communication technology, within the overall objectives formulated in the vision of the EC of a sustainable, ecological responsible, circular economy.
- Communication of these goals with all stakeholders
- Identification of the key road blocks in terms of scientific, technological, organisational, and economic aspects. Within the present context, special attention should be given to the aspects involving materials modelling.

- Formation of teams to develop strategies for overcoming each of these roadblocks
- Creation of mission-oriented, multi-disciplinary teams and implementation of the above strategies to achieve the specific goals
- Communication of the achievements to all stakeholders, i.e. dissemination of success stories
- Positioning the achievements to move the acquired know-how and technologies beyond TRL7

Concerning software, it has to be understood that academic software written by researchers during their doctorate or as post-docs is an initial step towards commercial software, but not the ultimate solution. While academic researchers have to be aware of the various stages of software from concepts and prototypes to mature, professionally supported industrial solutions, they need to concentrate on their strengths, namely to develop, explore and publish new theoretical and computational approaches and to position their creations for further development in the technology chain. For example, it may be more important to write a very clear documentation of the underlying computational approaches and algorithms with well-designed and documented test cases, rather than leaving a computer program, sophisticated as it may be, without sufficient documentation. Most likely, in the course of the life of software, the underlying concepts and algorithms will persist, but the specific code and programs will be refactored due to changes in the hardware, computer architecture, and programming paradigms. It should also be understood that only a small fraction of academic software will make it into an industrially successful software product, as is the case for many other R&D projects.

In summary, for the successful implementation of this Roadmap and the deployment of materials modelling software, it is critical that all players, industrial end-users, professional software suppliers, and academic researchers, focus on their domain, while working together as a team using a common ontological framework and strive for the highest level of excellence with the ambitions, to make Europe the leader in leveraging mankind's most powerful tool, namely computers and information technology, to achieve a sustainable, ecologically sound, and internationally competitive industrial eco-system.

7 Translation and Training for Companies

Industrial innovation requires access to professional players who have the ability to translate industrial problems into cases to be solved using modelling and simulation tools, namely, the Translators. These stakeholders should be able to promote and boost the innovation, playing a pivotal role in bridging the gap between the industrial end users, the software owners and the academic model developers. This role includes the need for bridging the "language gap" among the different stakeholders, in order to facilitate contact, collaboration and exchange of ideas. Thus, Translators should have a number of different skills, encompassing technical and economic aspects, besides soft skills. The credibility of the Translators is based on "neutral" support for the benefit of the client, independently of any personal or economic interest.

7.1 State of the art at present

Translation and Translators

A good basis in defining the role of the Translators and the components of the translation process has been set with the development of the Translators Guide (to be found at https://emmc.info). The

Translators Guide was created with the digested feedback from a large number of events and activities organised by EMMC. These include:

- Specific sessions on Translation at the EMMC workshop, April 2017 in Vienna
- Specific sessions at the EMMC Focused Workshop, June 2017 in Uppsala
- Survey on “Translation Cases”, April-August 2017
- Survey on “Industrial User Cases”, April-August 2017
- Survey on “Materials modelling Criteria for translators”, August-September 2017
- Focused workshop at the E-MRS Fall meeting, September 2017 in Warsaw
- Expert meeting on Translation, June 2017 in Eindhoven
- EC/EMMC Focused Workshop on Translation, September 2017 in Brussels

The translators guide is intended to be used by the Translators themselves for guidance and also by the industrial end users to know what to expect from the translators.

This guide can help translators when approaching industry, when defining/choosing the right modelling workflow and when defining the benefits of the modelling project. It gives directions on possible ways to execute transition. It is up to the Translator to decide/choose how to accommodate the guidelines described in this document. The choice depends, for example, on the type of industry and on the level of modelling required.

The generic components of the translation process include good understanding of the business and industrial case, analysis of the data available from the client, translation to modelling workflows, suggestions for the execution of the modelling project, proposing validation strategy of the models and when necessary, translation of the modelling results to information that is understandable and usable by the client. This back-translation, or interpretation of modelling and simulation results, needs to be adapted to the decision making process in industry and strongly depends on the way of decision making itself. While high-level management is initially mainly interested in risk assessments and business opportunities, which may be assessed using rough estimates, the level of detail necessary for the economic analysis of modelling and simulation activities require more technical tools for decision making by R&D people, such as KPI (Key Performance Indicators) models. Translators target to deliver not just modelling results, but a valuable and beneficial solution for the industrial problem!

The Translators Guide discusses also the specifics of the translation for SMEs, internal translation (mostly in large companies) and outlines some possible further actions that can be undertaken to ease the uptake of modelling in industry. By now, Translation cases from different type of translators and for different type of companies are currently not included in the Translator Guide.

<u>Training of Translators</u>

In order to perform the translation in the best possible way, the Translators need to possess a wide range of skills. These include knowledge (broad and deep) of modelling and experimental tools, data analysis, soft skills, industrial background, and knowledge on estimating the economic aspects and impact of modelling, credibility in justifying the choices proposed to the client for the use of certain modelling tools. Thus, the training of Translators is to be designed to encompass the above skills, which have been formalized along with the role of the Translators in the Translators Guide. Based on these considerations, training activities are currently being designed and planned.

Given that the EMMC-Marketplace (EMMC-MMP) will be the main repository for the online training material, the structure of an already available marketplace for the online simulation and training has been analysed: NanoHub[12]. NanoHub is an online platform for community-contributed simulation tools for science and engineering, with particular focus on nano-technological problems and applications. This platform provides the possibility to create interactive simulation tools, offers lectures, seminars, tutorials and discussion groups. Everything is accessible from the web browser and is free of charge. The EMMC-MMP will have a similar comprehensive role, storing online training material such as video-lessons, presentations and other documents as well as dedicated forums.

An initial set of training material has already been collected, in the form of lectures given by members of different modelling communities and by different industrial end users during modelling sessions at events and workshops organised by the EMMC. This training material will be expanded and made available on the EMMC-MMP. Training network should be also created and expanded. In a first step towards this goal, the EMMC Translation Group presented the plenary lecture at the International scientific event[13] and discussed the Translation aims, Translation process and RoMM (Review of Materials Modelling) as well as the MODA (Modelling Data) concept.

7.2 EMMC Ambition

We want to establish in Horizon 2020 the role of Translators as key players at the interface between manufacturers on the one hand and software owners and modellers on the other hand. Translators will support the usage of multiscale materials modelling in industrial R&D practice to the same level as experimental efforts are used today. The main topics handled by the Translators are a significant reduction of the language gap between manufactures and modellers, trustworthy KPI modelling on top of materials modelling and the integration of business oriented measures directly into the R&D process. This will broadly establish a new element in industrial R&D practice based on multiscale materials modelling.

At all levels of detail, Translators will need to provide and implement supporting tools for decision makers in order to answer “what if” questions based on the results of modelling and simulation workflows. The usage of validated models and tools within the workflows at various steps in the process is mandatory for Translators in order to build confidence in the materials modelling at the industrial work floor.

To facilitate and spread the Translators’ activities, a database of Translators need to be established. This database will contain information about the application domain and expertise of the Translators and their track record in translation cases. The database will be useful also for industrial users of modelling to choose the most suitable expertise/help in using modelling to solve (part of) their industrial challenges. The databases of Translators can be set-up at different levels, e.g. on the EMMC-Marketplace or other similar infrastructures.

Translation cases demonstrating the specifics (including bottlenecks) of the translation process for various types of industrial users (e.g. SMEs, large companies, different application sectors) need to be collected, shared among and used by the translators. These translation cases can form the basis of the track record of the translators.

[12] www.nanohub.org
[13] http://iwcmm27.be/prog.php

Translators will need to make use also of databases for different modelling/software tools and modelling/simulation executors (map of modelling expertise and tools). This database needs to be created by/with the help of modelling experts and software vendors.

Training of Translators

In order to translate the technical industrial problem to a modelling workflow, Translators need broad background knowledge of existing models and software and their capabilities. This core competence allows Translators to identify within the industrial (sub-) problems where modelling and simulation can really make a difference in terms of the quality attributes of a solution to be developed. The technical KPIs are modelled by the Translators as functional of the usually multiscale state variables of the physical/chemical modelling appropriate for a “good enough” simulation. Translators are not bound to specific models or software tools; they are **neutral** and do their best to identify the best possible tools to be integrated into a modelling workflow without being biased by any personal conflict of interest.

In this view, Translators should be trained on a multiplicity of skills, encompassing technical and economic aspects. From the technical point of view, translators should be trained to have a wide overview of the available modelling and software solutions, to identify the best technical solution for the client’s needs. This technical assessment should take into account the costs and perspective economic benefits based on the expectations of the client. Therefore, from the economic point of view, the Translators should be trained to have a good understanding of the possible return on investments (ROI), key performance indicators (KPIs), marketing strategies, etc. Besides technical and economic training, Translators may benefit of ancillary information related to the EMMC network activities, as for the example, the MODA[14]concept and a basic understanding of the EMMO (European Materials Modelling Ontology) structure for interoperability and integration. Training of translators to document/create clear and concise translation cases may also be envisaged.

The next steps of the EMMC in this framework will be to scrutinize and design the best strategies for the training of Translators based on the arguments discussed above. In this sense, the EMMC-Marketplace will have a key role as an online collector of training material and for the coordination of the trainers’/trainees’ community network.

7.3 EMMC Approach

In the short term, the EMMC is expected to clearly define the role of the Translators and the strategies for their training. In the long term, more specific actions are recommended, such as for example using Innovative Training Networks (ITN)[15] for “Training programs for new Translators”, in order to facilitate the establishment of this important new role in Europe.

The role of the Translators

A significant advancement towards the recognition of the role of the Translators has already been achieved with the development of the Translators’ Guide. Further refinement steps to work on in this direction have been identified to be:

- To set up a Translators database with individual information on expertise

[14] Modelling Data
[15] https://ec.europa.eu/research/mariecurieactions/about/innovative-training-networks_en

- To collect well-documented non-confidential translation cases demonstrating the translation process for big companies and for SMEs (successful and/or difficult cases)
- To use and share the above cases in the Translators' database as examples for best practices and to show bottlenecks which translators may encounter.

Training strategies

Starting from the developed Translators Guide, the goal is to develop training courses for the new Translators with a focus on how to use materials modelling, simulation tools and concepts for the economic assessment in order to support industrial innovation. Attendees of these training courses will be provided with methods and supporting tools which will allow them to enhance the usage of materials modelling for innovation in the European industry.

The definition of the training strategies for Translators is ongoing. On the one hand, the training network is being created and will be widened through the broad EMMC community. On the other hand, suitable material for the online training via the EMMC-Marketplace is being designed.

With regards to the training features, the main points to address will be:

- To define the specific topics for technical and economic training
- For technical training, to focus on tutorials, real cases, validation cases for specific models, simulation techniques, etc. Academic modellers and software owners will be asked to contribute and participate by providing procedures to estimate the accuracy, the limitations and the validation of their models and software.
- For the economic training, to focus on the cost evaluation of the modelling activities, return on investment (ROI), key performance indicators (KPI), Business Decision Support System (BDSS), and other useful elements for the business case analysis.
- Soft skills and additional useful topics, e.g. MODA (Modelling Data) tables and EMMO (European Materials Modelling Ontology) for interoperability.

For the online training material on the EMMC-Marketplace, the key points to address will be:

- To set-up the Translators' blog (and training platform)
- To make available documented Translation Cases
- To collect/request video-lessons on the different training topics
- To link the publicly-available training offered by Software Owners

In general, the EMMC network is producing a considerable amount of high-quality material in the form of presentations and (public) documents that can be collected and published on the EMMC website. Presentation and training sessions at events and workshops can be also recorded and made available in the form of video-lessons. Specific material for the online training could be also obtained by experts of the specific fields or academic Professors upon request. Besides this online training for Translators "channel" on the EMMC platform, the possibility to organize "traditional" training courses and events will be also considered.

8 Data Repositories and Marketplace: Material Knowledge and Open Innovation Platforms Information Management

8.1 Enhanced access and utilisation of repositories

The overarching goal of the EMMC in this domain is to establish leadership in increased utilisation of integrated materials modelling and data through radically enhanced collaboration and innovation platforms building on strong interoperability across all modelling fields.

Subfields of modelling as well as experimental science develop increasingly mature databases for their own fields. In these databases, both simulated and experimental data are gathered. While a *de facto* standard for data (including models, input and output) should make it easier to maintain such databases and leverage enough momentum for their use, internal structures and data formats are mainly driven by individual communities and the belief is that the subfield databases should remain structured as the subfield has designed them to satisfy their purpose.

Interoperability between data repositories has emerged in recent years as an alternative to such *de facto* standards on metadata. Similar to the interoperability between modelling tools and the development of EMMO [16] and various EMMO metadata schemas, interoperability between repositories can be achieved by developing standard reference API's and top level metadata exchange mechanisms. **However, such approaches have not yet matured enough to allow seamless exchange between all materials related data repositories.** For example, the Open Archives Initiative provides a protocol for metadata harvesting as a low-barrier mechanism for repository interoperability [17]. However, the metadata schema is not based on EMMO and is yet to be seen how it can be used or adopted by the materials community in general and the modelling community in particular. OPTiMaDe is an action that emerged from the electronic modelling community that is working in the direction of making electronic modelling and related databases interpretational by developing a common REST API, i.e., web based interfaces. NOMAD [18] has in recent years significantly advanced access and discoverability to electronic materials data and models by providing basic practical avenues based on metadata mapping.

Yet, there is a need to develop and agree on an overarching reference standard for the exchange and discovery of information and data in repositories without changing the internal structure and formats used by each subfield. Such a reference standards should cover all modelling subfields and applications.

Moreover, each field is still organised as an isolated data repository, largely isolated from other fields, gathering data remains largely unavailable to the other subfields and these subfields are until now not communicating enough. EMMC has coordinated with various data providers and is establishing a catalogue of repositories on the EMMC-Marketplace hub (on https://emmc.info) that aims to increase collaboration between various repositories and making them more discoverable across different communities.

[16] European Materials Modelling Ontology
[17] https://www.openarchives.org/pmh/
[18] http://data.nomad-coe.eu

Today, scientific results are published mainly in written form. Some publishers do allow a certain amount of supporting data. Nevertheless, the raw data itself is not available for further use and interpretations. And when this data is available, it is usually in rather native syntactic formats of the applications that produced them, and thus do not lend themselves easily for reuse. They require human intervention to create conversion tools to allow their utilisation outside of the original domain they are created in. Often these data are not complete or lack metadata completely and they are not machine-process able.

The EMMC is developing schemes that allow Materials Modelling to be documented using MODA[19] forms. An online version is available since end of 2017 and integrated into the EMMC-Marketplace at https://emmc.info allowing end users to document their modelling and actions to allow upload or linking to raw input and output data are being developed by the EMMC-Marketplace in tandem with Materials modelling Marketplaces IA in the EU. Such an approach significantly increases data sharing and promotes interoperability between modelling communities and repositories.

The long term goal is to establish an exchange/interpreter of databases that for a specific material gives e.g. the electronic structure, atomic nuclei positions, and particle/grain and continuum behaviour. This goal will pave the way to establish a holistic modelling approach and thus produce realistic predictions of materials behaviour under real world conditions. Key is that these subfield activities and databases will be co-ordinated so that available data become visible to all stakeholders in all subfields. A structured exchange should be generated and supported based on an exchange methodology to interpret and share the information in the different subfields. This should alleviate the current incompatibility or incompleteness of the set of distributed databases.

Another important aspect is addressing societal and technological barriers for sharing information. EMMC engages in coordination and support actions to raise awareness for curation of materials data and will drive the proliferation of repositories. Collaboration with various repository owners and data providers to envisage actions along these lines are vital.

8.2 Enhanced innovation through increased digitalisation of materials modelling

The overarching goal of the EMMC in this domain is to enable the increased digitalisation of materials modelling and provide efficient information and knowledge management for the benefit of the entire community.

The advancement of digitalisation, cloud and online technologies has brought many changes to our daily lives, both on professional and personal levels. New generations of scientists are constantly exposed to, grow accustomed to and become dependent on new online social networking and cloud tools as part of their normal workflows. They expect to be able to use the same tools for their future professional careers. For example, email, that emerged in the 80's to be the workhorse of team sharing and collaboration is being replaced by emerging instant messaging collaboration platforms (slack, Mattermost, etc.), (physical) library visits are replaced by online information platforms, and collaboration workflows are being created and executed online (cloud computing, HPC, and soon EU

[19] Modelling Data

Materials Modelling Marketplaces). The materials modelling community has been so far slow to adapt and take full advantage of the new online capabilities and the new avenues it offers to collaborate and conduct science online. **The digital single market initiative (DSM) of the EC calls for deeper digitalisation of materials modelling activities to enable more vigorous innovation in materials modelling and its tighter integration with the entire industrial value chain**. Emerging activities within Industry 4.0 call for additional actions that allow materials modelling to be more discoverable, usable, and Integrate-able with the overall digitalisation actions in Europe.

This can be achieved by an all-encompassing online presence of materials modelling activities via a Materials Modelling Marketplace Hub that collates all related activities in Europe and provides a one-stop-shop for all the needs of all stakeholders, from modellers, translators, educators, business decision makers to industrial R&D. **Such a hub becomes a place for information exchange on key issues concerning materials modelling and its industrial application**.

Such a platform needs to be supported in med-term and long-term actions such as open innovation hubs or which are platforms that create additional integration of modelling related services and workflows as well as experiments into the existing Marketplaces and extending them.

There is a lack of such a platform that is focused on exploring possibilities of-, and offering novel solutions to the entire European materials modelling community. There is a need not only to create such hubs, but to also **actively create and populate these Marketplace hubs with content** in the form of materials modelling services for models, translation, education and networking. The creation of the corresponding **informational environment and infrastructure** is crucial for a smooth and rapid transform of the contemporary and future scientific knowledge and modelling experience to the industry (and thus to the society in general).

The insufficiency of information exchange between the areas of fundamental materials modelling and their potential end-users are at present one of the major obstacles for further progress of material science. The other major, and possibly most critical obstacles are the intrinsic limitations of current theoretical and computational approaches to capture the complexity of industrially relevant materials and processes. **There is therefore an overarching need for a vibrant innovation platform that manages the materials modelling infrastructure and provides content including integrated materials modelling, translation, education and data repositories and that caters for all application domains and subfields, i.e., electronic, atomistic, mesoscopic and continuum.** A Materials Modelling Market Place bringing together and integrating information and databases and libraries of models and data, validation and educational resources fills this need.

However, actions to populate these emerging platforms with content and providing use cases to demonstrate how to utilise these novel paradigms are needed. Such platforms should be open innovation platforms or hubs that assists and further strengthens R&D foundations in Europe ensuring its continued leadership in advanced technology and modelling. **Such actions also need continuous development and are expected to morph with time to address the most pertinent requirements of industry, modellers, translators and educators.**

8.3 Enhanced collaborative science and enabling transfer platform: the future of Materials Modelling Marketplaces

The overarching goal is that Materials Modelling Marketplaces provide a central innovation hub for materials modelling activities in Europe, including Training and Translation services for Manufacturers. Materials Modelling Marketplace platforms provide information technology infrastructure for deeper integration of materials models, development of workflows and access to concerted data repositories and collaboration platforms for the benefit of all stakeholders.

The EMMC envisages strongly connected communities of various stakeholders, which have easy access to a Hub that provides for a vibrant digital collaboration tool with databases (of data and knowledge). The platform would also contain a model selector that helps select the right set of workflow components and a set of experimental data to validate the models in the new specific application (and therefore can be used by Translators and integrated in a BDSS[20]). This would be completed with an explicitly named contact individual from the software owner who is responsible for producing and maintaining the model.

Materials modelling Marketplaces act as a digital online Transfer Platform that will address key technological, organisational and human capital gaps. The underlying main concept stems from the recognition that bringing materials modelling benefits to manufacturers requires a new collaborative and integrative approach that reaches out through the limits of each modelling or manufacturing community.

The Modelling Market Place (Materials Modelling Marketplace) is **a platform** of integrated components that leverages modern information technology paradigms to:

- Connect the relevant actors and stakeholders
- Connect modelling communities and components
- Enable Big-data material informatics and analytics
- Facilitate collaboration and open information exchange including best practice, validated methods and information about approaches that have been found to be unsuccessful, or insufficient, for certain cases
- Establish collaborative science paradigms in support of materials modelling in industry

The latter would be immensely useful to expose model deficiencies, and hence drive new needs and actions for specific model enhancements and new model development that will be critical for a successful implementation of materials modelling in industrial problems.

The Materials Modelling Marketplace contains not only databases but also other intangible resources such as education, expertise exchange, communication platform, etc., that are linked with the databases, allowing therefore easy mapping of raw and interpreted data with corresponding stakeholders and experts. It will facilitate **Big-Data schemes** to be employed and integrated into a Business Decision Support Systems (BDSS) by manufacturers and translators. See Figure 4 **Fehler! Verweisquelle konnte nicht gefunden werden.** for the structure and contents of the Materials Modelling Marketplace.

[20] Business Decision Support Systems

The Materials Modelling Marketplace allows industry to collaborate with Translators and modellers in more efficient ways to create integrated materials modelling solutions that collate various modelling and data expertise to address pertinent industry challenges in a timely manner.

8.3.1 Unified access to databases and the Big-data challenge as an enabler of materials informatics

Materials Modelling Marketplace provides unified seamless access to disparate data repositories. The various repositories are envisioned to be more than just a collection of data repositories; they also include knowledge regarding the models used and workflow to obtain them. It is necessary to keep these components alive by continuously updating and linking them to changing resources (expertise, case studies, etc.). Materials Modelling Marketplace can become a **gateway to materials modelling and its "big-data".** Collating repositories and providing unified access creates a critical mass of data necessary for Big-Data and data mining. Systematic data mining (e.g. by artificial intelligence, model reduction, quantitative structure/activity/-property relationships, etc.) represent a promising approach for fully exploiting the potential of collected (Big-) data.

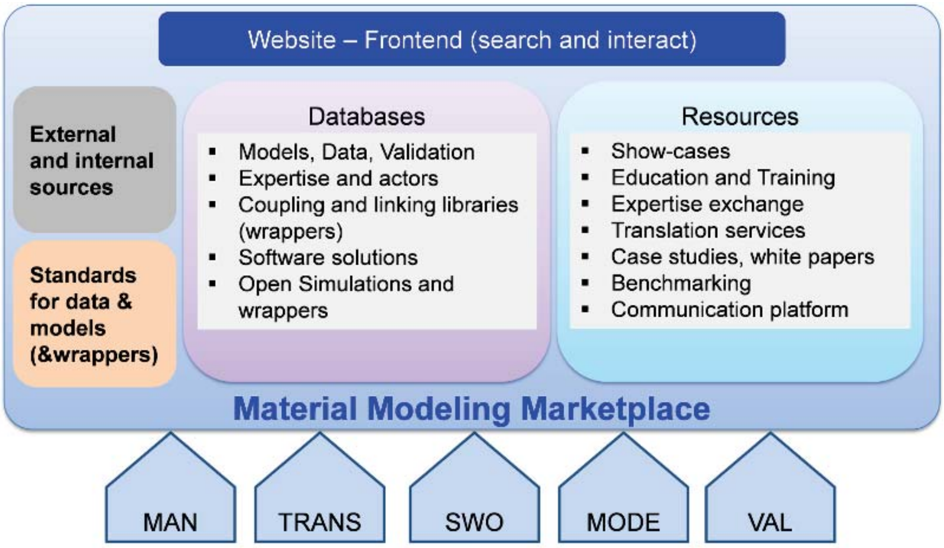

Figure 4 A schematic structure of the various components in the Material Market Place and relation to stakeholders

8.3.2 Provisions for intellectual property (IP) and privacy management

The requirements to protect intellectual property still needs to be adequately considered. One example would be the distinction between competitive and non-competitive data. The first may have additional constraints on storage and retrieval within the Materials Modelling Marketplace. The degree of openness of the data in the Materials Modelling Marketplace will be determined by the owners and the goal is to provide schemes to allow for a fine-grained control of the level of data openness to be made. However, a more open data sharing model will significantly contribute to the establishment of a sustainable eco-system for the benefit all stakeholders.

8.3.3 Coupling & Linking workflows and open simulation platforms on the Materials Modelling Marketplace

The Materials Modelling Marketplace enables coupling/linking of all components in and effective, easy and maintainable way. Standards and ontologies are needed for optimal information management, retrieval and interoperability of different components. Common ontology is expected to immensely enhance the effectiveness of retrieval, archiving, exchange and reuse of the data. Coupling and Linking (C&L) of models often need novel physics and chemistry, which is usually part of the post-processing in the MODA[21] workflows. Hence C&L models need to be developed and wrappers (interface software) are needed for models and databases to talk to each other and these can be developed based on the new ontology based standards (EMMO[22]-schema). Schemes to allow any modeller, translator or educator to incorporate their models and expertise to provide them as a service on the hub as part of open simulation platforms should be provided. **EMMC Marketplaces are to be seen as bare-bones-bazars that provide an open integration platform for both vendors and end users to collaborate and conduct science online**. Bare bones bazar means that the platform is open to any third party providing services, offering tools, building integrated workflows, and providing translation and education services. The Marketplace platform itself provides the needed connectivity to host such resources as well as providing front end access to end users seeking to utilise such services.

8.3.4 Validation of models

The Materials Modelling Marketplace also enables data quality to be tested and validated against experimental data using automatic means (artificial intelligence). Figures of merit (confidence level) and other measures need to be agreed with the stakeholders. Furthermore, the Materials Modelling Marketplace will make it possible to publish data, models and early results. Each such publication on Materials Modelling Marketplace will have a unique identifier that can be cited.

8.4 Increased utilisation of materials modelling in industry and benefits to all stakeholders

The wide availability of Market Place hubs providing access to a wide range of information on materials modelling and as well as possibilities for collaboration and communications will accelerate and advance materials modelling design and deployment in the EU. It enables more vigorous utilisation of integrated modelling and data in the industrial value chain leading to rapid developments of new products and materials. Sharing of technical information, i.e., expertise, data repositories and standards along with advances in IT presents an **immense opportunity** for the modelling community, manufacturers, and software owners in EU. Materials Modelling Marketplace provides new avenues for all stakeholders to collaborate and conduct business transactions online supporting both software owners and modellers by bringing added value to industry end users.

8.4.1 Benefits to Manufacturers (MAN) include

- Accelerated development of materials modelling solutions, especially ICME
- More validated models and means to find information rapidly breaking through geographical or community barriers
- Direct access to all materials modelling expertise and resources in the EU
- Mapping of available modelling activities and resources in EU

[21] Modelling Data
[22] European Materials Modelling Ontology

- Readily identify needs for modelling, data and expertise
- Access to translators and model developers services
- Ability to distinguish between validated and not validated models and degree of validity of various models

These benefits are expected to lead to a strong decrease of time to market and costs of development of new products.

8.4.2 Benefits to Software Owners (SWO) include

Given the complexity of accurate and reliable materials modelling software, it is fair to assume that not a single software owner or software company will be able to offer all capabilities required for complete, multi-scale modelling in every application domain. For every SWO it is important to increase their visibility and to reach a wider market. Thus, the benefits for SWO will include:

- Higher competitive visibility in the market
- Better cooperation with suppliers of software with complementary capabilities
- Clearer understanding of the competitive landscape
- Earlier identification of modelling gaps, i.e. opportunities for introducing new capabilities in line with actual market requirements
- Convenient access to Translators

8.4.3 Benefits to Translators (TRANS)

For TRANS, the Materials Modelling Marketplace offers a valuable resource as well as a channel for education and communication with MAN, repositories of best modelling case studies, white papers and best modelling approaches and standards. A requirement that the TRANS stakeholders have for Materials Modelling Marketplace is that it offers:

- A direct communication channel with MAN
- Databases of models, software tools and materials data and uncertainty.
- Databases for case studies, white papers and webinars
- Ability to connect modellers and models to MAN for providing solutions
- Creating solutions both online on the Materials Modelling Marketplace platform and offline
- Access and collaboration with SWOs

8.4.4 Benefits to Modellers (MOD)

Materials Modelling Marketplace will also provide value to MOD in a number of ways, including:

- Vibrant online collaboration platform to develop advanced modelling workflows
- Increase access to their modelling expertise and tools to allow wider exploitation
- Enhance dissemination in the academic simulation community
- End users can publish and access modelling results using the databases and show cases
- Each publication on Materials Modelling Marketplace will have a UUID/URI (unified universal ID, universal resource identifier) or DOI
- Keep track of citations with eventual publication (link UUID to DOI)
- Publish results before finalizing a paper: get cited more and early, increase competitiveness and collaboration

- Speed of outreach: reduce development time of new products
- Allow data to be reused: sustainable use of resources
- No peer review, internal ranking based on use (hits, downloading, etc.) and user feedback
- Higher impact of modelling in manufacturing

8.5 State of the art today

The current state addressing the question of “Where are we today” can be summarised as follows:

Marketplaces and repositories are an emerging action in the EU with much anticipation for specific levels of services by the entire community. There is a need therefore for the EMMC to closely coordinate with all stakeholders promoting further the development and utilisation of Marketplaces on the one hand, and interacting with existing projects and actions to devise practical ways to address current and future expectations and needs and building content on the Marketplaces and materials repositories on the other.

Materials modelling Marketplaces are a novel undertaking on the EU level. The EMMC has promoted and initiated the concept of Materials Modelling Marketplaces in its previous roadmaps as a response to clear and strong stakeholder’s demands. As a result, a call topic in NMBP 2016[23] program was established for the creation of such hubs that cater for the needs of all stakeholders. This has resulted in two new projects starting 2017 that shall provide the basic infrastructure and mechanism encompassing all tangible and intangible components needed to accommodate various core services for the benefit of the entire industry and all stakeholders.

Materials modelling Marketplaces is a novel concept as no such platform that augments collaboration, translation, education for industry, materials modelling services as well as catalogues of data repositories exists. The EMMC has a goal to support these emerging activities further and coordinate and network with these actions in the EU to ensure their compliance with the demands of the community as depicted in its previous and current Roadmaps and updated from continuous feedback collected by means of EMMC online discussion forums, workshops, online surveys and direct interaction with all stakeholders. Especially, towards this end, providing common communication avenues between all key players involved in Marketplace activities and in all related actions in the EU is of vital importance.

A significant recent advancement is the creation of the EMMC-Marketplace (on https://emmc.info) as a neutral central gateway and hub to all existing and future data repositories and Materials Modelling Marketplaces. The EMMC-Marketplace will soon contain basic elements for collections (i.e., catalogues) of educational resources, industrial case studies, translator resources and networking activities. These need to be developed further to provide direct input from the community building dynamic collections of software repositories and catalogues of repositories with metadata. The aim is that the community will create and add content to such catalogues. In addition, the EMMC coordinates with existing materials data repositories in order to facilitate their cataloguing and access through the Marketplaces.

[23] NMBP-25-2017: Next generation system integrating tangible and intangible materials model components to support innovation in industry

8.5.1 Current feedback and needs

Further targeted feedback from the community on the actions pertaining to needs and requirements for Materials Modelling Marketplaces and data repositories was obtained including the following direct inputs from the community via:

- Specific sessions on Marketplaces and data repositories at the EMMC workshop, April 2017 in Vienna
- EMMC survey on Discussion points for the EMMC International Workshop 2017
- Specific sessions at the EMMC focused workshop, November 2017, Cambridge, UK
- EMMC Survey of materials modelling development needs 2016

At this point of time, Materials Modelling Marketplaces and data repositories are on an important cusp of change. Marketplaces are just starting to be set out and a number of materials modelling data repositories exist. While no Marketplaces are actually available yet, apart from the initial version of the EMMC-Marketplace, and no widely agreed and adopted interoperability between data repositories exists, **this Roadmap aims at providing forward looking actions based on community feedback that are meant to accompany the development of the Marketplaces and set out grounds for their future utilisation.**

The most pertinent feedback resulting from the EMMC networking actions are:

1. Industry clearly re-iterated its need for a Materials Modelling Marketplaces with data repositories as means to increase the use of materials modelling in industry in general.
2. Common interoperability interfaces are needed to facilitate unifying access to scattered repositories and increased discoverability and integration in Marketplaces.
3. Marketplaces provide tangible avenues for developing and including Integrated Computational Materials Engineering (ICME) workflows into the industrial value chain.
4. Allow industry better management of information and knowledge, initially from materials modelling, but a link to characterisation is anticipated at a later stage.
5. Provide rapid avenues to materials data from simulation as well as experiments for validation and as input to materials models and for easing materials selections.
6. Better curation of results and as means to preserve, maintain and grow knowledge within the company.
7. As means to foster more rapid communication and networking with Translators, educators and modellers. In particular the notion of "chat rooms" and discussion forums was brought forward.
8. Helping industry to find the right information about materials, models, modellers and translators.
9. Need for common access, or common interfaces (application programming interfaces, APIS) for disparate repositories.
10. Clear guidelines and practical solutions for IP protection and privacy measures are vital.
11. Guidelines and practical solutions for benchmarking and user feedback are needed such that it allows constructive interactions.
12. Sustainability of Marketplaces and data repositories as a critical issue that will have to be solved before companies can rely on such services.
13. There is a need for use cases to demonstrate the benefit and use of Marketplace and connections to disparate repositories.

14. Interoperability between repositories, modelling tools, and information and materials data in general is an important aspect that will promote increased utilisation of Marketplaces.
15. There is a need to avoid fragmentation and "re-inventing" the wheel, by coordinating with existing related actions and repositories and all stakeholders integration paths so as to create a single hub for Marketplaces and data repositories without limiting the development of individual platforms.
16. Sustainability of Marketplaces and data repositories in the long run is crucial so as to allow industry to adopt them.

The feedback from all stakeholders demonstrates that Materials Modelling Marketplaces are emerging and there is a strong need from the community to get them active as quickly as possible and augment them with services that allow their demonstration and use by all stakeholders. In particular, IP issues, privacy and user feedback mechanisms require concerted actions between all Marketplaces, repositories and related activities with the EU DSM to devise services that address stakeholder needs and demands and comply with the DSM objectives.

The need for Big-data analysis and Deep Learning (including Analytics and artificial intelligence methods) in the Marketplace platform was also clearly requested. The databases and integration are seen to be highly ranked by industry. As such there is a need to foster Big-Data and Deep Learning on the emerging Marketplaces.

8.5.2 Current related actions

In tandem with the actions of the EMMC, few other initiatives have led to platforms that have certain similarity with, and share the global vision of the EMMC Marketplaces, most notably MaterialsCloud, NOMAD, Fortissimo, MAX, and others in Europe and nanohub.org in the US, which mostly target data repositories, modelling and education services for the electronic and atomistic communities. The EMMC coordinates with these and other similar actions towards better integration to cover all models and industrial sectors.

The NOMAD repository (https://nomad-repository.eu) hosts currently over 44 million entries of materials property calculations using state-of-the-art ab initio quantum mechanical approaches. This is an example of a major successful project funded by the E.C. In fact, this repository is becoming one of the world's largest and most comprehensive repositories of its kind. The Materials Market Place will leverage this accomplishment and put it into a wider context.

8.6 EMMC Ambition

The overarching goal is to populate the materials marketplace innovation hubs with content allowing demonstrating their use in the first step, and increasing the participation of the community in the next step. Marketplaces require active participation of the entire community!

The ultimate goal is to create and maintain online vibrant platforms that collate all services needed for increased utilisation of materials modelling in industry. Existing and emerging platforms need to be filled with content in the form of models, translation and education services, software solutions and linked databases of data and expertise. As seen from the previous section, there is a need to encourage and stimulate wider participation in the emerging Marketplaces in the form of content creation and consumption. There is a strong need to support information management and exchange in an open way that still preserves IP rights for industry. Databases and integration of workflows is a dominant factor requiring interoperability within and between Marketplaces which demonstrates the relevance of the EMMO (European Materials Modelling Ontology) for marketplaces and data repositories and further demands agreement on common APIs and interfaces between Marketplaces and within Marketplace and repositories.

In summary, industry and all stakeholders require addressing the following issues in the current stage:

1. IP protections
2. Sustainability and long term longevity of repositories and Marketplaces
3. Augmenting Marketplaces with apps and usable services
4. Demonstration and use cases

8.6.1 Secure platforms and authentication

The future Marketplaces should be online hubs that provide users (both vendors providing services, and end users consuming such services) an open platform that has solid IP and privacy protection, and provides critical mass of services, including materials models, repositories, integrated simulation platforms, and translation services. The EMMC will accompany the existing actions with the EMMC-Marketplace (hosted on https://emmc.info) to provide a common hub, and an early testing ground for various services to collect feedback from the community.

There is a need to investigate possible avenues for IP protection and devise means to address them. The goal is to allow each stakeholder, especially from industry, to be able to conduct online transactions without compromising their IP. A mix of open and closed business models will address this issue, at least partially. Marketplaces must provide open API allowing industry to interact with Marketplace services from behind firewalls providing various levels of privacy control.

Authentication services are key for IP protection. The goal is to allow better, preferably interoperable authentication between various repositories, marketplaces and the EMMC-Marketplace allowing each Marketplace hub or repository to cater for more users that just those that happen to register to one Marketplace or repository. This is foreseen to immensely provide for larger common user base and enable more streamlined IP management and boost interoperability between Marketplaces and repositories in general. Collaboration with the EC, DSM, and DGCNECT actions is a prerequisite here.

8.6.2 Self-sustainability and longevity

The goal is to create avenues for self-sustainable Materials Modelling Marketplace hubs and repositories linked to EU infrastructure (storage and CPU/HPC providers) that supports businesses and all stakeholders for the long term.

Data repositories and Materials Modelling Marketplaces must have clear business models to facilitate long-term sustainability of services. This requires both the development of business models as well as deeper interaction with infrastructure projects that can provide necessary resources for long term storage of information and knowledge as well as CPU cycles for modelling services.

Better and closer collaboration with European Open Science Cloud (EOSC), EUDAT, OpenAir, and other DGCNECT actions is a goal. Achieving self-sustainability requires increased active participation of all stakeholders. It requires a critical number of vendors and end-users to have an active online presence, i.e., registered active users and conducting modelling and related business on the hub so as to generate sufficient revenue to enable maintaining services at a high level of quality for the benefit of all stakeholders.

There is a need to provide CPU cycle services for Marketplaces and a link to EU HPC infrastructure. Such a link should provide better authentication of users and services for utilisation of EU HPC from within Marketplaces. Standards for authentication and IP protection have to be developed.

8.6.3 The bare-bones-bazar paradigm

Marketplaces provide an open platform allowing any stakeholder to develop exploitation avenues and use marketplaces for the benefit of the entire community.

The bare bones bazaar concept means that the Materials Modelling Marketplace does not contain built in materials modelling workflows, translation, or any other service, apart from the needed framework that allows any stakeholder to bring its own services to the marketplace. Metaphorically, MaTerials Modelling Marketplaces provide the “booths” only, and the entire community provides the actual content and innovation on top of the marketplace.

There is an overarching need to convey the scope, goals and targets of Materials Modelling Marketplaces. Especially clarifying that Marketplace hub is to act as open, bare-bones-bazar that is open to any stakeholder to act as vendor providing services on the platform, or as end consumers of services. For this, an agreement of standards for interfaces and data based on EMMO[24] is required, so that vendors can easily and more efficiently integrate their services. This is a vital issue to allow the population of Marketplaces and repositories with content and services needed for their successful utilisation in industry.

There is a need to make all available and future services integrate-able in one Marketplace hub. To this end, the EMMC works with current and future actions to agree on means to achieve such integration seamlessly. This requires the development and agreement on a set of reference interfaces and data representation by means of ontologies and standards. Future actions, including the emerging EU Marketplaces need to devise and agree such standards based on EMMO to allow integrating all needed services, including data repositories. It should be noted that an integration to one hub does not mean one online platform, but rather refers to the integration of services provided potentially, by many online platforms.

8.6.4 Use Cases, workflows and population of Marketplaces with content

Industry requires Use cases to demonstrate and educate on how to utilise such Marketplaces and data repositories in the value chain. Such use cases can start from the simple using initially basic services such as those hosted on the EMMC-Marketplace. However, the efficient demonstration requires substantial services to be available on the Marketplaces.

Therefore, actions that cater for content generation, i.e., integrated modelling workflows, open simulation platforms, materials data repositories, translation and educations resources, materials repositories and other tangible and intangible services into the Marketplaces are needed.

Current Materials Modelling Marketplaces actions in the EU target various use cases that have various levels of complexity and at least some cases are expected to be ready by 2018-2019. However, the

[24] European Materials Modelling Ontology

EMMC-Marketplace can be used to target use cases that are based on use of basic translation services and data repositories access. While such use cases do not demonstrate the full potential extent of services and use cases possible, it acts as initial demonstrations that can induce further interactions from industry and translators.

Basic scenarios for use cases can also be devised based on other exiting actions. They should utilise the EMMC-Marketplace repository of Translators and software solutions to search and find translators and/or solutions and/or repositories, use the online contact functionality to initiate contact with respective experts or repositories/solutions and start a case study offline. When online modelling services are available then the same use cases can be adapted accordingly.

Other use cases can also make use of existing services developed by BDSS[25] projects or other online platforms (NOMAD, OPTiMaDe, FORCE, etc.).

8.6.5 Discoverability and interoperable repositories

Increasing the discoverability of repositories can immensely benefit from a central catalogue with high level metadata providing a searchable directory of repositories and general description of their content in the first level. The EMMC has already collected an initial set of such repositories, and these will be published on the EMMC-Marketplace. The aim is to allow users to contribute content to the catalogue as well.

The goal is to provide first a catalogue of what exists, and then to provide unified access to all repositories content provided interoperability interfaces included metadata are agreed upon. In the first stage links to material data repositories that are relevant to materials modelling (such as for input) and calculated data are to be supported.

8.7 EMMC Approach

The Materials Modelling Marketplace and data repositories require input and involvement from all stakeholders. Materials Modelling Marketplace development will rely on input and collaboration with manufacturers to guarantee that the above mentioned resources and databases comply with their needs and therefore be of best practical use in the long run to the entire industrial sector in Europe. Interoperability between repositories based on EMMO[26] and common reference interfaces will enable databases to "talk" to each other. The involvement of the SWO in this is critical. Translators would assist in identifying the intended audience of Materials Modelling Marketplace; this makes a huge difference in the appearance of, for instance a web page. Translators should also get involved in actions of the Materials Modelling Marketplace.

Actions that promote the generation of content and linking existing content into the emerging Marketplaces are of utter importance. In addition, a common reference standard for the easy integration of services and content onto the Marketplaces is of great importance too. The EMMC-Marketplace can act as a test ground and common platform to develop and test such components (where the main development work is done in the IA and RIA projects). The EMMC-Marketplace can be used to test in particular various education, translation and networking components. An example are the discussion forums and "social media" components already integrated in EMMC-Marketplace based on existing open source technologies will provide initial valuable input to existing Marketplace projects in the form of feedback from the community to provide improvements on the

[25] Business Decision Support Systems
[26] European Materials Modelling Ontology

existing. Additional work should be directed towards agreeing a community standard for the communication between data repositories and Marketplaces. These may be established in a CWA[27] workshop.

Additional awareness raising campaigns on the importance of data sharing and use of marketplaces will immensely help to attract sufficient participation in Marketplaces from both vendors and end-consumers. To this end, the EMMC dedicates one of its forthcoming focussed workshops and will utilise the EMMC-Marketplace Blogging channel as well as discussion forums to this end.

Collaboration and coordination with HPC centres and EOSC are important to allow Marketplaces to harvest EU infrastructure for CPU cycles and data warehousing. In particular, authentication schemes must be investigated in relation to privacy and IP protection will be conducted by the EMMC-Marketplace working group.

Initial content that relies on existing components (mainly open source) on the EMMC-Marketplace is planned to demonstrate various aspects of the Marketplaces, these include:

1. Repositories of MODA[28] and MODA portal
2. Software solutions database
3. Repositories catalogue
4. Educational and translators (experts) databases
5. Modellers and experts databases

These services are to be implemented such as to allow the community to create and add content, and at the same time provide user feedback on the correctness of the content.

Short and Mid-term actions:

1. Open Translation environment that utilises the marketplace platform to create and demonstrate the translation services (RIA)
2. Open Innovation Platforms for materials Modelling Workflows (RIA) to boost the creation of integrated materials modelling workflows including integration with experiments, validation and uncertainty estimates is needed

Mid and Long-term actions

3. CSA action and RIA to bring together EU Materials Modelling Marketplaces, open translation environments, test beds and innovation platforms including characterisation to large scale EU infrastructure for HPC and data repositories to enable one **true single digital marketplace for innovation in Europe.**

[27] CEN standardisation Workshop Agreement (CWA)
[28] Modelling Data

9 Interoperability and Open Simulation Platform

9.1 State of the art today

9.1.1 Context

Materials Modelling is well established in leading materials and manufacturing companies and a wide range of methods including those based on discrete (electronic/atomistic/mesoscopic) models are used. There is also an increasing integration of people/communities and insights from different domains and sub-disciplines (i.e. less of a discrete/continuum divide) at innovative companies. This leads to an increasing demand for the ability to really connect and integrate a wide range of models. Moreover, the drive towards a more integrated and digitalised R&D enterprise is leading to the demand for stronger integration and easier mining across data across all types of data source, be it modelling or experiment.

However, all stakeholders of materials modelling face barriers regarding access to, and use of, information about materials modelling, utilisation of the wide range of modelling tools and methods, and last but not least interoperability of models and codes.

Industrial problems can only be solved using several materials models together and there is a need to orchestrate the interplay of different models as well as corresponding software tools. In addition, the interoperability with databases (both experimental and simulation) needs to be further developed. The trend towards stronger integration means that materials models and related data are used more widely along the value chain. Today there is still a strong divide between materials modelling done at the discovery and development stage leading up to so-called material selection for product development.

However, there is an increasing drive in leading organisations to improve the integration of materials data and materials modelling across the enterprise, see for example the Boeing patent on the Product Chemical Profile System[29].

9.1.2 Materials Modelling Interoperability

The issue of interoperability refers to “the ability of computer systems or software to exchange and make use of information”[30]. In materials modelling there is often the need to link models in order to address typical industrial problems. Interoperability can be achieved by different means and on different levels, from syntactic (data format) definitions that enable ‘import/export’ via integrated platforms that operate on the basis of a certain ‘data model’ to semantic level interoperability. Today, most interoperability solutions in materials modelling work at the syntactic level. There are, however, a number of approaches to improving interoperability under way. One can call them ‘pragmatic’ in that they include some level of data organisation (e.g. using the hierarchical file format HDF5) and metadata schema limited to certain domains.

[29] https://materialsmodelling.com/2016/02/08/boeing-is-moving-ahead-with-integrating-chemistry-and-materials-modelling-into-the-product-life-cycle/
[30] https://en.oxforddictionaries.com/definition/interoperability

One of the most advanced attempts in this direction in a materials modelling sub-discipline has been the Chemical Mark-up Language (CML) development in the field of chemistry, electronic and atomistic modelling[31,32]. CML provides support for most chemistry, especially molecules, compounds, reactions, spectra, crystals and computational chemistry. In particular, the effort extended to dictionaries and semantic web tools.

The electronic structure and atomistic modelling community has also been advancing metadata and schema through a number of initiatives (some involving experimentalists) including those of (T)COD[33], NOMAD[34], ETSF[35], or the Pauling File[36]. To enable reproducibility, metadata should include provenance, which can also be used to generate metadata for any schema. Automated provenance tracking and metadata exporters[37] are included in AiiDA[38].

A number of 'software packages' (typically proprietary) provide some level of integration within one platform. The integration may be limited to a common visualisation/graphical user interface. Typically, there is also further interoperability, e.g. in atomistic modelling packages, different codes can operate on the same atomistic structure. As a result, these platforms support linking of certain models. However, linking is often limited to models of the same entity type (e.g. different atomistic models).

Open API integration and workflow environments are designed for easier and more flexible integration of codes, and for developing, managing and executing workflows. Examples of existing (open and proprietary) integration and interoperability environments include ASE[39], AIIDA[40], MuPIF[41], DREAM.3D[42], KNIME[43], Pipeline Pilot[44], MedeA®, AixViPMaP[45], Salome[46] and Simphony[47].

While all of the above software solutions are in some way pertinent to materials modelling, they have been developed with a wide range of different objectives and they don't share any common basis in the semantics of materials modelling. Hence, current approaches lack generality (as far as materials modelling is concerned) and are dependent on adhering to particular formats and metadata. It means that tasks for the materials scientist requiring to go across typical domain boundaries can be laborious and error prone. This observation was backed up by replies received to an EMMC survey and workshop discussion on interoperability.

[31] http://www.xml-cml.org/
[32] http://www1.gly.bris.ac.uk/~walker/CMLComp/
[33] Gražulis, S., Merkys, A., Vaitkus, A., Bail, A. L., Chateigner, D., Vilčiauskas, L., Cottenier, S., Björkman, T. & Murray-Rust, P. (2014). Acta Cryst. A, 70, C1736., http://crystallography.net/tcod/
[34] https://metainfo.nomad-coe.eu/nomadmetainfo_public/info.html
[35] http://www.etsf.eu/fileformats
[36] http://paulingfile.com/, http://developer.mpds.io/#JSON-schemata
[37] A. Merkys, N. Mounet, A. Cepellotti, N. Marzari, S. Grazulis, G. Pizzi (to be submitted)
[38] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, Comp. Mat. Sci. 111, 218-230 (2016), http://www.aiida.net/
[39] https://wiki.fysik.dtu.dk/ase/
[40] http://www.aiida.net/
[41] https://sourceforge.net/projects/mupif/
[42] https://immijournal.springeropen.com/articles/10.1186/2193-9772-3-5
[43] https://www.knime.org/
[44] http://accelrys.com/products/collaborative-science/biovia-pipeline-pilot/
[45] https://www.aihitdata.com/company/0135BDC3/AIXVIPMAP/overview
[46] http://www.salome-platform.org/
[47] https://github.com/simphony

The community deals with the need for interoperability and integration in a variety of ways today. Some points from a recent EMMC survey and discussion at the EMMC International Workshop 2017 are shown below.

> *There is **no systematic approach**; each workflow is different: e.g. based on either simple approaches (parameter passing and surrogate models) or transferring, manipulating complex data files. Interoperability is often done by **import and export of data based on certain formats. Some software provides proprietary common data format, some open, standardized data formats**, such as VTK or HDF5 are also used widely. **There is no semantic framework in place**. Integration is done e.g. on the programming **API** level or with manually developed translating **files**; **JSON APIs** translations in C++. Such specific solutions can be **very efficient, but they are not general**. APIs avoid the need to make any change in the simulation software tools to be added to the interoperability environment, which allows an **easy extension to new applications**. However, the interoperability remains on a syntactic level. This means that it **relies on particular metadata (e.g. HDF-based) as common interchange format**. No semantic information is yet included in the implementation.*

An important step towards facilitating interoperability for Physics based models has been taken recently with a CEN standardisation Workshop Agreement (CWA) on Terminology, Classification and Metadata for Materials Modelling. Based on the Review of Materials Modelling (which itself is based on the analysis of well over 100 FP7 and H2020 projects over many years), the CWA provides (a) concise definitions for the key high level terms in materials modelling, (b) a classification of physics based models (by entity, then Physics Equation and subsequently Materials Relation) and (c) a standardised documentation of all aspects of simulations, covering the user case, model, computational representation and post-processing.

It provides the basis for further development of a solid semantic foundation for materials modelling. Other fields of science and technology, e.g. genomics and bioinformatics have made great strides organising their knowledge and enabling collaboration across a wide range of stakeholders by developing such a semantic foundation in the shape of ontologies. An **ontology** is a formal naming and definition of the types, properties, and interrelationships of the entities that really or fundamentally exist for a particular domain.[48] Ontologies aim to define which entities, provided with their associated semantics, are necessary for knowledge representation in a given context.[49] Ontologies and related information technology provide an opportunity to share a common understanding of the structure of information within a specific domain, the possibility to reuse domain knowledge, to make domain assumptions explicit and to analyse domain knowledge.[50]

In response to these needs and challenges, the EMMC has spearheaded the development of the European Materials Modelling Ontology (EMMO). EMMO is designed to address the needs for a semantic description which is deeply rooted in Materials Science, incorporating:

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[48] https://en.wikipedia.org/wiki/Ontology_(information_science)

[49] Thomas R. Gruber (1993). Toward principles for the design of ontologies used for knowledge sharing. Originally in N. Guarino and R. Poli, (Eds.), International Workshop on Formal Ontology, Padova, Italy. Revised August 1993. Published in International Journal of Human-Computer Studies, Volume 43, Issue 5-6 Nov./Dec. 1995, Pages: 907-928, special issue on the role of formal ontology in the information technology

[50] David Lamas, Metadata and Ontologies, 2011; https://www.slideshare.net/davidlamas/metadata-and-ontologies

- A description of materials from a rigorous physics perspective.
- Formal relations between granularity levels to facilitate multiscale materials description.
- Definition of material processes to capture the changing and evolution of materials as chain of different states.

These features provide a natural framework for expressing our knowledge about materials science including in particular the interrelation between process, structure, property and models.

9.2 EMMC Ambition

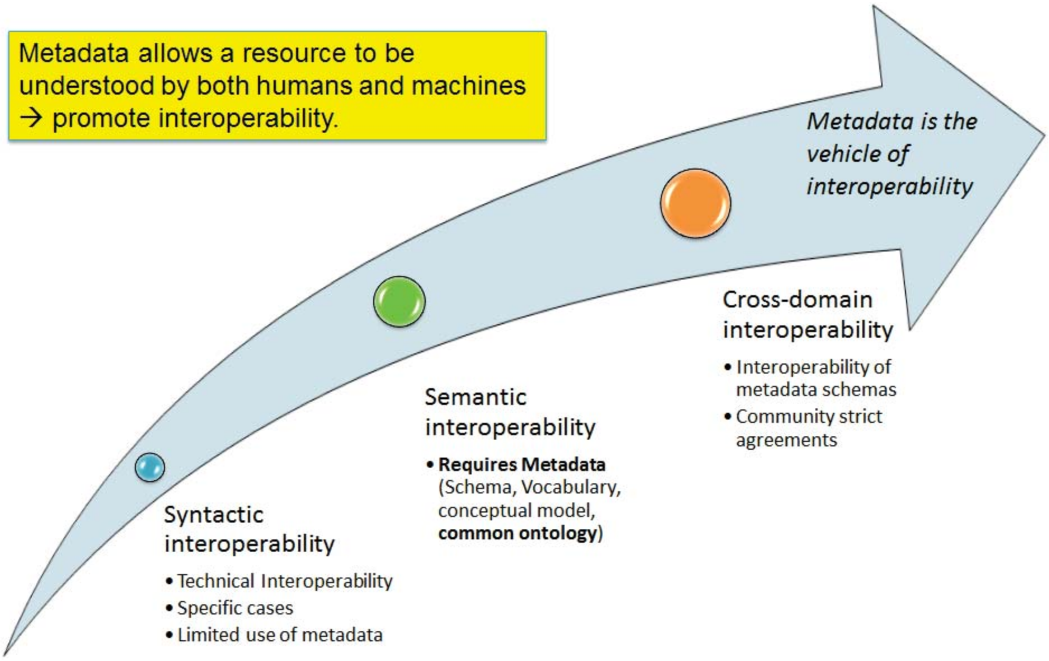

Figure 5 Interoperability

In order to drive the fourth industrial revolution (Industry 4.0) in the materials related sectors, materials data and models need to become highly integrated and interoperable. The term Materials 4.0 has been coined to paraphrase the digitalisation of the material, supporting the whole value chain from discovery and development to process, production, service life and recycle. Materials 4.0 will enable materials to be understood and utilised as variable systems with tuneable properties.

Faster, wider and deeper take up of digital technologies in the materials and manufacturing industries will provide additional value by supporting the development of digital marketplaces and hubs, faster and more agile materials development, new business models, use, re-use and improved life-cycle management of materials, energy and resource efficiency, addressing societal challenges and competitiveness of European industry.

In this context, the task of the Modeller will be more strongly integrated in the enterprise, interoperability and integration are required to serve such functions as integration into business decision support systems, digital marketplaces, translation environments, and more generally innovation hubs that connect technologies and data from a wide range of disciplines, in particular characterisation and manufacturing. Interoperable systems will be able to respond to varying demands on simulation workflows and data management.

We can identify a number of materials modelling related goals and objectives along the road to achieving Materials 4.0 and eventually Industry 4.0. In this regard it is useful to consider all the elements of a Simulation, i.e. the complete set of activities needed to arrive at a calculated answer to a user question. As documented in the MODA, it involves the User Case, the computational representation of the Physics Equation as well as the Materials Relation and of course, the input data as well as post-processing into certain output properties. It also includes workflows that may involve linking and coupling of models.

Firstly, to provide a basis for such semantic interoperability, a fully-fledged and tested European Materials Modelling Ontology is required. The development of EMMO is relevant for an integrated technological development and brings benefits for industrial end-users in terms of common understanding and improved communication, knowledge management, consistent data interpretation and linking of resources, advanced search, inferencing and reasoning providing answers to queries that would otherwise remain unanswered. It will facilitate digitalisation of materials and manufacturing and the enable powerful Artificial Intelligence applications. The wide range of reasons for ontologies and benefits of ontologies includes common understanding, data interpretation, source linking, establishing and enforcing rules, inferencing capabilities reasoning also across data sources (hence answer queries that would not otherwise be answered) etc. However, currently there are a wide range of efforts and approaches ranging from fundamental ontologies to purely application-oriented ontologies that are not based on fundamental physics/materials science concepts. There is therefore a clear need for one common ontology across the materials field to enable knowledge extraction and exchange was clearly endorsed by the audience.

The ambition of EMMC is to push for and facilitate further development, wider integration and application of the European Materials Modelling Ontology.

Secondly, an Open Simulation Platform (OSP)[51] built on the basis of EMMO will greatly facilitate workflow generation and execution by humans and machines, i.e. by modellers, by translators and in semi-automated systems such as Business Decision Support Systems, Open Translation Environments, Open Innovation Platforms and Digital Marketplaces.

An OSP facilitates putting all these pieces together in order to carry out a simulation based on semantics, and with definitions/standards that are independent of specific implementations. In particular it should be straight forward to combine physics equations with materials relations and also straight forward to source and read in data for the parameters of those relations for specific materials. Given a Simulation 'plan' that has been worked out by a Translator to tackle a certain User Case, the Modeller should therefore be able to implement the simulation in an efficient and effective manner. The plan and the outcomes of the simulation will be documented with metadata (based on EMMO) in a way to support data mining and analytics as well as enable others to reproduce the simulation, both using the same codes and using different codes implementing the same models. It will hence be straightforward to replace one code by another in a given workflow. Beyond the 'single' user case, the

[51] In OSP, Open refers not to open source software but denotes the openness of the semantic foundations.

management of complex workflows requiring either machine or human decisions would be supported by such a platform.

The ambition of EMMC is to push for and facilitate the development of an Open Simulation Platform the enable a seamless and standardised integration of all simulation aspects, including the representation of the material, any type of physics-based models (including different materials relations), solvers, pre- and post-processors and databases. OSP will be based on existing and emerging standards for semantic interoperability across domains.

9.3 EMMC Approach

European industry can play a leading role in driving the digital revolution, but this requires a much more long-term sustainable approach to utilising data and modelling. It must involve coherent and compatible semantic foundations and standardisation. Cross boundary developments that integrate vertical industries and digital providers must become the norm[52]. Therefore, also interoperability needs to be regarded as a challenge that is shared by all sectors, not just materials modelling. Related challenges are managing interfaces between different domains and systems, data exchange and data ownership and digital trust. Lessons should be learnt from other sectors who are transforming, including banking, pharma and insurance. For example, there is a similarity between materials and pharmaceuticals in terms of the workflow and divide between the stages pre- and post-selection (see Figures 5 and 6). Pharmaceutical companies also recognised that they need to improve integration of information and knowledge across these stages in order to speed up development and avoid late stage failures. The sector has been very active and forward looking in the development of semantic frameworks and ontologies (see Batchelor, Allotrope etc).

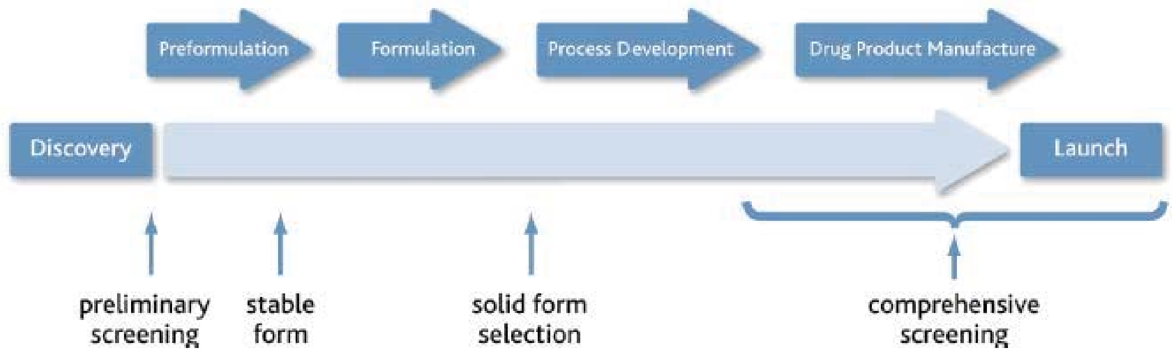

Figure 6 Active Pharmaceutical Ingredient discovery and development workflow

The long-term goal of achieving cross-domain interoperability based on a semantic framework will take some time to achieve.

Building semantic foundations requires ontologies (i.e. a controlled vocabulary for representing the types of entities in a given domain) covering the different fields (domains) that are relevant to a simulation. Following the MODA, this means the User Case including of course the materials and processes to be simulated, the (physics-based and data-based) models, the computational representations and the pre-and post-processing operations. Furthermore, the domain ontologies need to be built in a coherent way such that they support reasoning without conflicts and ideally in a

[52] CEN/CENELEC Workshop: Standards for Transformation, Workshop Output Summary, 2016-06-30.

way such that they share common roots. Unless a common approach to building ontologies is used, the effort in building semantic foundations will lead to just another range of incompatible sub-disciplines.

The goal of the EMMC is to coordinate and support efforts of building 'systems' or 'platforms' which are able to support all of the above requirements on a flexible and unifying manner. We can learn from the experience in other fields, which have dealt with the issue of organising the collaboration and integration across a wide range of disciplines and stakeholders (e.g. systems biology, genomics, analytical instrumentation/Allotrope, etc) that building an integrated platform with such a wide range of capabilities (integrating different types of models, codes, handling different types of user cases, workflows, database interactions etc) requires a solid and unifying semantic foundation[53].

The task is to utilise the standardised terminology and classification already agreed in the CWA[54] and build formalise it into a taxonomy and ontology of materials modelling. Such an ontology can form the basis for formal metadata development with which models and databases can be linked. These developments would further support efficient solutions for modelling and the communication, dissemination, storage, retrieval and mining of data about materials modelling.

Ontologies are however not sufficient in themselves to achieve an Open Simulation Platform (OSP). Low-level tools are necessary to support communication between models and to verify integration (in low-level, programming and high level, semantics of variables, constraints and phenomena). These tools should be consistent with common ontologies.
Also, once an ontology is available and full semantic interoperability thus is achieved, the next challenges to be addressed relate to timing and conditions triggering the information exchange and to respective decision-making tools being assembled along with the models in flow chart type simulation ecosystems.
In the end, the expectation is for "a set of full turn-key simulation work-flow driven solutions for industrially-relevant practical problems."

In order to achieve the above goals, the following objectives should be targeted.

(1) The adoption of a widely agreed terminology and standardised documentation of Materials Modelling to support communication as documented in the CWA needs to be further supported in a wide range of communities.
(2) The EMMO as a basis for cross-domain semantic representation requires further development, integration with other disciplines (e.g. integration between materials modelling and characterisation as well as manufacturing, targeting in the end an integrated digital representation of materials along the value chain), as well as a formal governance framework.
(3) Agreement on and development of a platform that is based on the ontology and enables increasing levels of interoperability: an Open Simulation Platform (OSP), where Open refers not to open source software but denotes the openness of the semantic foundations.
(4) Putting an EMMO based semantic framework and OSP at the heart of Marketplaces, Open Translation Environments and Business Decision Support Systems.

[53] Sreedhar Reddy, B.P. Gautham, Prasenjit Das, Raghavendra Reddy Yeddula, Sushant Vale, and Chetan Malhotra. "An Ontological Framework for Integrated Computational Materials Engineering." In Proceedings of the 4th World Congress on Integrated Computational Materials Engineering, 69–78, 2017.
[54] CEN standardisation Workshop Agreement

10 Model Quality, Model Development and Model Validation

The overall focus of the model development and validation action within the EMMC is the identification of m*odel gaps in industrially important sectors, and how to widen the models in an appropriate way for industrial needs.* Here strategies for the *coupling and linking of models* is becoming increasingly important. Equally important are the needs to *validate the models and workflows*, *verify their quality and applicability* in the context of their intended use. The EMMC thus has four main actions in the area of model development and validation, namely (i) identification of model gaps and strategies to overcome them (Section 10.1), (ii) best protocols for coupling and linking of models (Section 10.2), (iii) model verification (Section 10.3), (iv) and model validation (Section 10.4).

10.1 Model gaps

10.1.1 EMMC Ambition

European materials-based industries need access to state-of-the-art models and modelling workflows of increasingly high quality, reliability, and descriptive (or predictive) power in order for computational materials modelling to have a significant impact on their procedures and strategies. To achieve this we need to, on the one hand, promote the improved and wider exploitation of *the best existing* models and workflows, and on the other hand, promote the *development of better* (and yet computationally feasible) models that will enable a more realistic description of complex materials and their functionalities. Model and method development activities need to be enhanced in a forceful, focussed and sustainable manner, and targeted towards the current and future needs of industry benefitting from it.

In short the main goals of the development action of the EMMC are

- to identify model gaps in industrial applications,
- to promote the use of discrete particle-based (electronic/atomistic/mesoscopic) models in industry for the added value that they *per se* provide, as well as for integrating them with continuum models to connect the gap to macroscopic matter.

10.1.2 EMMC Approach

Networking and consultation with a wide community of current and future modelling stakeholders are key components for a successful endorsement of our Roadmap on "model development beyond existing gaps". Our work until now has proceeded in a systematic fashion as follows.

- From “EMMC Survey of materials modelling development needs: discussion notes towards the *Road Map 2018-2020” (May 2016; publicly available on the EMMC web site*): Automotive and chemical applications combined represent more than half of the total feedback, followed by energy, and then metallurgical including the aerospace sector. Within the automotive applications, the dominant secondary application is metallurgical, followed by chemical applications. Within the chemical applications, energy storage (batteries), metallurgy and electronic applications were the most prominent secondary applications.

- Three meetings with a focus on model gaps were held in the first half-year of 2017, namely two targeted sessions at the *EMMC International Workshop 2017 in Vienna* 5-7 April 2017, and two EMMC meetings held back to back in Uppsala in June 2017, namely the *Focused Workshop on Model Quality,* *Gaps & Accuracy* in Uppsala 15-16 June 2017,[55] preceded by an open meeting addressing *discrete models and C&L strategies.*[56]

- The collated results of the surveys and the informed discussions and presentations at the three meetings, we proposed to elaborate on model gaps in the following sectors: *Automotive/aviation metallurgy*, *Microelectronics*, and *Chemistry & energy*, which we decided to split into *Heterogeneous catalysis* and *Interfaces* (functional materials, energy materials, composites and soft matter/polymers). Pharmaceutical crystals were highlighted at the Focused workshop in June and after taking into account opinions from the nano-safety community the pharmaceutical manufacturing & nano-safety topic was shaped. After taking into account comments from the Commission that the Coal and Steel Programme is catering to the modelling needs within the automotive/aviation metallurgy sectors we propose the following five topics. Whether further refinements or extensions are needed will crystallize out in the subsequent endorsement process. Thus, the elaboration of model gaps within the following five sectors will be currently in focus.

(S1) Heterogeneous catalysis,

(S2) Microelectronics including organic electronics,

(S3) Interfaces (e.g. functional materials, energy materials, composites),

(S4) Molecular matter including polymers,

(S4) Pharmaceutical manufacturing & nano-safety.

These sectors display a large consistency with the WP 2018-2020 NMPB calls.

10.2 Coupling and linking of different models

10.2.1 EMMC Ambition

The idea of modelling general materials properties at the electronic level is still a (very) distant possibility and is furthermore a very inefficient *modus operandi* in terms of required computing power. In coupling and linking (C&L) workflows, models of a lower granularity benefit from information available at a underlying more fine-gained level. This is the coupling and linking or multiscale process. A note about our terminology is in place here: Within the EMMC we prefer to avoid the word “scale” as it might imply that the main difference between the electronic, atomistic, mesoscopic, continuum classes is one of system or problem size, while in fact the difference is more multifaceted (*see the RoMM VI publication*[57]). However, the term multiscale modelling is deeply rooted within the area of C&L; thus, we use the terms quite interchangeably within this chapter, in order to make this document as much as possible understandable to a wide modelling community.

The 2016 survey indicated that C&L models is of a high priority for industrial stakeholders. Currently C&L workflows are developed with specific material types and physical/chemical processes in mind. A common approach is needed if C&L models are to engender confidence in the industrial user base. Now it is recommended to move towards a formal C&L approach which incorporates the best features in terms of the purely computational aspects of information exchange, for example detail of data

[55] https://sites.google.com/view/emmc-uppsala-june17/

[56] https://sites.google.com/site/ emultiscale2017/

[57] https://publications.europa.eu/en/publication-detail/-/publication/ec1455c3-d7ca-11e6-ad7c-01aa75ed71a1

structures, while preserving the physical basis of the models at all granularities. Within this context our aims are

1. Create an overview of C&L techniques by material type.
2. Facilitate a discussion forum around basic C&L approaches in expert workshops and related conferences, such as the International Conference on Multiscale Modelling (http://mmm2018.jp/).
3. Draw up recommendations for generalised C&L approaches.
4. Supporting the required interoperability of relevant codes and producing recommendations of open source platforms for automation of the C&L process.

10.2.2 EMMC Approach

The multiscale materials modelling is continuously under development, and given the high diversity of materials and of their numerous conditions as well as the diversity of available C&L approaches, a reasonably unified approach would be needed on a long term. Moreover, industrial stakeholders will require indications that the added effort of C&L approaches, compared to traditional models, are worthwhile. So far, contacts have been established with a number of relevant organizations and groupings with competence in C&L strategies at the European level, such as CECAM[58]/ECAM and the modelling-oriented Centres of Excellence. Roadmaps and strategies developed at the international level are being examined, such as the initiatives taken by NIST[59], with its particular focus on the Materials Genome Initiative (MGI)[60] as well South Korean initiatives are of interest; both were represented at Multiscale modelling meeting arranged in Uppsala in June 2017. The MODA (Modelling Data) datasheets collected by the EMMC will be helpful towards identifying relevant stakeholders in the C&L framework, and feedback will be collected from such stakeholders on best-available C&L methods for industrial use.

10.3 Verification – uncertainty quantification

Definitions - Verification and validation. The terms verification and validation are often used interchangeably. It is suggested to adopt the following definitions (which is consistent with ISO 9000 industrial standard for quality management systems):

- Verification is the evaluation of whether or not a product, service, or system complies with a regulation, requirement, specification, or imposed condition. It is often an internal process. On the other hand, validation is the assurance that a product, service, or system meets the needs of the customer and other identified stakeholders. It often involves acceptance and suitability with external customers.

This means that, while the two procedures may have common features, verification refers to the internal checks which a model development group will apply to their code, whereas validation is a more 'outward looking' process aimed at the industrial customer. These definitions are a standard adopted by the IEEE.[61]

[58] https://www.cecam.org/
[59] https://www.nist.gov/
[60] https://www.mgi.gov/
[61] "IEEE Guide--Adoption of the Project Management Institute (PMI®) Standard A Guide to the Project Management Body of Knowledge (PMBOK® Guide)--Fourth Edition". p. 452. doi:10.1109/IEEESTD.2011.5937011.

10.3.1 EMMC Ambition

One of the characteristics that a model should have to be defined as "good", is its accuracy. In this sense, it is important to first clarify what we mean with accuracy. In general, an accurate model can be defined as one that provides correct predictions. However, no model can provide 100% exact predictions of reality; therefore, it is necessary to quantify its error (or uncertainty), that is, to define a procedure to measure its accuracy with respect to the expected results. In this view, the model verification is the procedure that allows to check that the model complies with the planned design specifications. With the above definition, verification can be seen as an internal check, which can be performed during the model development phase (on the whole model or part(s) of it) and/or at the end of the development. Here we shall focus on the design of methodologies for model verification, that is, design of reliable and systematic procedures for uncertainty quantification in materials modelling. With this purpose, we shall review the best available methodologies for error estimates in materials modelling, to allow definition of best practices for error quantification. It is also necessary to investigate the "systematic errors", which arise for example as errors in, or badly chosen, DFT functionals, errors in MD force-fields, and errors as a consequence of unphysical coarse-graining procedures. They often constitute the most serious model barriers and a significant reason why modelling results may be considered low in relevance for the industrial community.

10.3.2 EMMC Approach

The first stage in the procedure is to collect and analyse the different approaches adopted by the many actors in the field. We established interaction and collaboration with the NanoHub [62] platform. NanoHub already integrates specific tools for uncertainty quantification, see for example [63] the PRISM Uncertainty Quantification (PUQ)[64]. In further exchanges, information about NIST/NanoHub activities on uncertainty quantification in materials modelling have been collected. Model accuracy, including uncertainty quantification, was one of the themes of the focussed workshop in Uppsala (Sweden) in June 2017. We also keep contact with the Collaborative Computational Project on Computational Magnetism (CCP-MAG)[65] in the UK on model validation and error estimates.

10.4 Validation

10.4.1 EMMC Ambition

EMMC will propose standards and guidelines for industrial validation of materials models. Interaction with relevant European actions will be pursued in concert with ongoing and future LEIT calls to endorse the guidelines. One of the tools to accomplish this task will be the EMMC expert meeting during "*Workshop on verification and validation practices*".

[62] https://nanohub.org/
[63] https://nanohub.org/groups/uq
[64] http://c-primed.github.io/puq/
[65] https://www.ccp-mag.ac.uk/

10.4.2 EMMC Approach

The goal of defining standards and guidelines for materials model validation must proceed via the following stages:

1. Investigation of the current formal approaches to validation in general
2. Determination of the appropriate form for materials model validation in collaboration with the main actors, predominantly Software Owners (SWO) and external industrial stakeholders
3. Recommendation of a standard approach to materials model validation

Preliminary investigations have been carried out, resulting in a discussion document for consideration by the main actors. It is suggested that data-based models could be included in the same approach, which is important because data-based models can be based on data produced by physics based models. As such including data-based models in the validation process would subject them to similar standards and procedures.

11 EMMC Associate Measures

Introduction

Besides capturing scientific theoretical concepts in materials models, ensuring validity, accuracy and precision of model simulations, the connectivity on multiple scales of models, the combination of models with experimental data, making models available, the aid to implementation and using translators, connecting materials models with other business information, and model integration into existing business environments, there is the important issue of **Infrastructure and Digital Aid Algorithms**.

Infrastructure

On Jan 24, 2018 Microsoft CEO Satya Nadella stated at the World Economic Forum in Davos, Switzerland that the world is rapidly ”running out of computing capacity” as “Moore’s Law is kind a running out of steam”. Materials modelling for the most complex problems requires significant computational power. Although not necessarily part of the objectives of the EMMC to address this issue the effort in place and planned for the future will heavily depend on the availability and access of existing hardware. Europe needs to ensure it remains at least in pace with the latest developments and significantly contributes to potential resolutions of this issue. For example, quantum computing is considered as a potential path forward. Such developments require the attention of the materials modelling community in terms of the way models are conceived and used, and certainly in the ways they need to be implemented for industrial purposes. A close interaction with hardware development of modellers is therefore to be stimulated.

Depending on the type of models and complexity of the problems to solve and were materials modelling can assist a significant investment in hardware may be required. Easy access to Distributive Computing, Cloud computing and HPC facilities may be a requirement. However, with companies this will raise the important issue of security and confidentiality that needs addressing in a convincing fashion. Investment in own computational facilities typically bring new challenges and significant investments that smaller companies are not prepared to make or can afford. Software owner and translators may need to offer besides expertise and materials modelling tools equally the ease to implement and use the provide services. This calls for new business models possibly aligned to the Open MarketPlace approaches. Furthermore, infrastructure needs maintenance and upgrading as technology progresses.

Digital Aid Algorithms (DAA)

Digital Aid Algorithms is a catch-all phrase for all the algorithms required to enable materials models to be used. This includes topics from tailored graphics user interfaces to multi-variable optimisation routines, to API's for querying databases, to a multitude of small or major "calculation" algorithms. As an analogy, a car comes to mind as a functional tool that essentially requires an engine to do the job of transportation. However, the car will be useless and impossible to be handle without the multitude of utilities from steering wheel, brakes, clutch, wheels, seats, gas, and so on, not to mention a certain level of driver skills to control and master the car even if the "driver" is replaced by a collection of sensors. A significant effort should be put in place to ensure these DAA are made available along the materials model "engines".

In fact, the development of sophisticated simulation software is an industry all in itself and Europe has the opportunity to capture this opportunity and to become a world leader, especially in the field of materials modelling software. However, the highest level of professionalism will be required to achieve this ambitious goal and to reap the economic benefits for the European tax payer.

11.1 Industrial Integration and Economic Impact Associate Measures

Following actions are proposed:

- Ontology development and governance
- Data-based and physics-based model integration

11.2 Industrial Software Deployment Associate Measures

Following actions are proposed:

- Building on the data, knowledge, and material acquired by the activities of the EMMC, organise events such as workshops and leverage the online Forum to keep all stakeholders related to the industrial deployment of materials modelling software informed about trends and to network all players.
- Stimulate research and educational institutions to foster multi-disciplinary curricula and research projects, as is done, for example, within the Doctoral Training Centre at the materials science department of the Imperial College in London.
- Foster programs to expose young scientists and engineers to industrial problems and challenges, for example by ITN's and secondments.
- As an important pillar, promote and support mission-oriented innovation hubs with the goal to solve prototypical and specific problems by an integrated, multi-disciplinary approach combining advanced experimental synthesis and characterisation with the whole range of state-of-the-art modelling technology including physics-based and data-driven approaches. These innovation hubs would thus become prototypes for the integration of the best available materials R&D tools (experimental and computational) for addressing specific topics. Possible specific objectives include additive manufacturing of high-performance materials, organic and nano-technology-based electronics for sensors and display, spintronics, advanced energy

storage systems, materials for extreme conditions (e.g. fusion reactors) as well as many other possible applications.

- The integrated technology emerging from the innovation hubs can serve as models for bringing these solutions in house, which would be interesting for large industrial manufacturers, and they can evolve into centres serving SME's.

11.3 Translation and Training for Companies Associate Measures

- In the short term, the EMMC is recommended to develop the role and functioning of Translators. In the long term, an Marie Skłodowska-Curie Innovative Training Networks (ITN) is recommended for a "Training Program for new Translators" in order to facilitate this important new role within Europe.

11.4 Data Repositories and Marketplace: Material Knowledge and Information Management Associate Measures

Short and medium-term actions

Continue current EMMC-Materials Modelling Marketplace actions:

- MODA portal with search facility
- Software solutions databases,
- Repositories catalogue,
- Experts and modellers databases,
- Educational and translation resources (case studies, translator guides online)
- Discussion forums
- Experts profile, registration and elementary authentication
- Initial draft agreement with repository owners and data providers on common interoperability between repositories
- Possibly initiate a CWA for interoperability standard between repositories dependent on feedback from all stakeholders and the EC
- Creating links between MODA portal and raw data in repositories as well as experts and translation repositories on EMMC-Marketplaces
- Expert Group meetings with IA Marketplaces to agree integration of services

Medium and long-term actions

- A Coordination and Support Action (CSA) is needed for assembling and coordinating activities starting from 2019. The CSA should take on the role to actively stimulate participation in the database activities.
- RIA and IA projects that contribute content in the form of modelling services, data repository access, data, translation services, educational services and other relevant content to existing marketplaces
- RIA and or IA actions to create more case studies and use cases for existing Marketplace hubs

In the CSA and RIA actions:

- Design of tools for interpretations of raw characterisation data
- Requirements and Design of tools for validation of models including constitutive equations
- Case studies with examples on how these databases function for dissemination

11.5 Model Quality, Model Development and Model Validation Associate Measures

11.5.1 Model gaps

For our subsequent endorsement process we will make use of two novel ingredients that were introduced, namely (i) a novel workflow to identify industrially crucial model gaps and (ii) a novel concept *qualified industrial end-user* (Q-MAN). The Q-MAN is a stakeholder with the following characteristics: user of materials simulation tools (modelling and R&D knowledge) *and* employee of an industrial company (having knowledge of their applications). We will identify a large number of qualified Q-MANs and collect their experiences and viewpoints about model gaps via surveys or individual interviews. The action culminated in the "Expert Meeting on the promotion of discrete materials models in industry" in Torino in February 2018. In more detail, the plans are as follows:

1. Select a large number of SWOs involved in discrete modelling to help us find Q-MANs.
2. Perform surveys/individual interviews with the selected Q-MANs.
3. Digest all the comments from the qualified industrial end-users and forward them to expert meeting (anonymously).
4. Arrange an expert meeting on the promotion of discrete models in industry in February 2018.
5. Further elaborate the feedback towards the white paper, roadmap and training material for the new procedure.

11.5.2 Coupling and linking of different models

EMMC will continue working on the identification of the model gaps, focusing specifically on the screening of the available Coupling & Linking (C&L) strategies. The theoretical, computational and hardware limitations of the currently-available C&L methods will be determined, to aid the identification of best strategies. This is an ambitious task given the diversity of material types, each having its own unique C&L approach. Synergies from collaboration with the Interoperability and Integration teams of the EMMC will be exploited. Specific actions are

- Analysis of the diversity of C&L approaches and formulation of recommendations concerning strategies for viable workflows and model interoperability, including potential universal approaches.
- We will (i) collect MODA from existing projects; (ii) identify the C&L steps and (iii) contact C&L stakeholders.
- A C&L expert meeting will be held to present initial results and plans for continued identification of the industrial needs for the multiscale approach.

11.5.3 Verification – uncertainty quantification

The best available techniques for uncertainty quantification will continue to be scrutinized, and their suitability for application in materials modelling assessed. This activity will lead to establish best practices for quantifying error estimates in the framework of materials modelling. Specific actions are

- A best-practice guide for standardizing the error estimates of materials models will be elaborated based on the collected case studies
- The most significant ones will become pilot studies, to be published on the EMMC website

- Characterising the systematic errors in e/a modelling and preparing guidelines for translators on appropriate approaches for specific material types
- A modelling verification best practice guide will be developed (report in August 2018). This best-practice guide will be synchronized with the European Materials Characterization Council

11.5.4 Validation

- Carry out a systematic analysis of validation methods.
- Consult with SWO to determine at least a generic model of their approach to validation.
- Work towards a standard procedure for materials model validation.

Document History

- *V3.02, first release on 2015.2.26, last revision on 2015.4.20: slight revision of the Translation section, moving section 7.2 further up, and minor typos.*
- *V3.0.1, first release on 2015.2.26, last revision on 2015.4.14*: is based on a revision of Version 3 on 14.4.2015 to include a table of contents, shortening and clean-up of the Translators sections: 4.2, 6.2, 6.3, and 7 and including the previously missing Figure 2.
- *Following extensive discussions within the EMMC and a special meeting in Brussels on the 4th of January 2015 the consolidated and endorsed roadmap was finalized and published on the EMMC website on 26.2.2015 (Tagged as V3)*
- *The first draft of the roadmap was released by the EMMC on 22.12.2014 with contributions from all EMMC working groups.*
- *V1.0.6, first release of the EMMC RoadMap 2016 was released by the EMMC on 27.09.2016, latest revision on 2016.11.21.*
- Updated version of the EMMC RoadMap 2018 is based on wide stakeholder consultations in a large number of EMMC organised/co-organised workshops, expert meetings, online surveys (e.g. EMMC International Workshop 2017, EC/EMMC Translation Workshop, EMMC Workshop on Interoperability of Materials Modelling, EMMC Workshop on Model Quality, Gaps & Accuracy, EMMC Business Decision Support System Expert Meeting etc.)