The European Materials Modelling Council

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Abstract The aim of the European Materials Modelling Council (EMMC) is to establish current and forward looking complementary activities necessary to bring the field of materials modelling closer to the demands of manufacturers (both small and large enterprises) in Europe. The ultimate goal is that materials modelling and simulation will become an integral part of product life cycle management in European industry, thereby making a strong contribution to enhance innovation and competitiveness on a global level. Based on intensive efforts in the past two years within the EMMC, which included numerous consultation and networking actions with representatives of all stakeholders including Modellers, Software Owners, Translators and Manufacturers in Europe, the EMMC identified and proposed a set of underpinning and enabling actions to increase the industrial exploitation of materials modelling in Europe. EMMC will pursue the following overarching objectives in order to bridge the gap between academic innovation and industrial application:

- enhance the interaction and collaboration between all stakeholders engaged in different types of materials modelling, including modellers, software owners, translators and manufacturers,
- facilitate integrated materials modelling in Europe building on strong and coherent foundations,
- coordinate and support actors and mechanisms that enable rapid transfer of materials modelling from academic innovation to the end users and potential beneficiaries in industry,
- achieve greater awareness and uptake of materials modelling in industry, in particular SMEs,
- elaborate Roadmaps that (i) identify major obstacles to widening the use of materials modelling and (ii) elaborate strategies to overcome them.

Keywords: Materials Modelling, Models, Coupling / Linking, Interoperability, Metadata Schema, Open Simulation Platform, Marketplace, Validated Software, Data Repositories, Translation, Economic Impact

1. Introduction

The development of new and improved materials is a significant **innovation driver** for the global competitiveness and sustainability of European industry and society in general. It has been demonstrated in many individual cases

that **materials modelling is a key enabler of R&D efficiency and innovation**. Companies reported [1] that computational modelling benefits include reduced R&D time and cost, more efficient and targeted experimentation, more strategic approach to R&D, a route to performance optimisation, wider patent protection, improved supply chain control and early understanding of application performance aiding faster and more assured market introduction. **Nevertheless modelling today is still not always an essential part of or critical tool in creative materials design or business decision making on product innovation**. Thus, the overarching goal of the **European Materials Modelling Council (EMMC)** is to stimulate and enhance the use of materials modelling in industry, in particular SME's. It implies fostering ongoing efforts, addressing observable hurdles, enhance the visibility, inspire improved models and step up the contribution of materials modelling to strengthening the global competitiveness of the European manufacturing industries and complementing the drive to the fourth industrial revolution, known as Industry 4.0.

The aim of the EMMC is to establish current and forward looking complementary activities necessary to bring the field of materials modelling closer to the demands of manufacturers (both small and large enterprises) in Europe. The ultimate goal is that materials modelling and simulation will become an integral part of product life cycle management in European industry, thereby making a strong contribution to enhance innovation and competitiveness on a global level. Based on intensive efforts in the past two years within the **European Materials Modelling Council (EMMC)** which included numerous consultation and networking actions with representatives of all stakeholders including Modellers, Software Owners, Translators and Manufacturers in Europe, **the EMMC identified and proposed a set of underpinning and enabling actions to increase the industrial exploitation of materials modelling in Europe** (Fig. 1).

Fig. 1. The different enabling and underpinning activities of the EMMC.

The EMMC will build on these findings by supporting activities such as open¹ simulation platforms, information infrastructure, materials marketplace and business decision support systems, databases, multiscale coupling science, education and translation activities and validation. **Our vision is that only when considering all these elements together sufficient synergies can be created to address the most challenging questions and overcome the hurdles for further industrial application of materials modelling**. In particular this will enable manufacturers to utilise modelling in their business decisions, much as this is done today with experiments. This will help close the innovation gap (“valley of death”) between materials modelling and industrial application and enhance a knowledge driven product development process.

2. EMMC Objectives

EMMC will pursue the following **overarching objectives** in order to establish and strengthen the underpinning foundations of materials modelling in Europe and bridge the gap between academic innovation and industrial application:

1. **Enhance the interaction and collaboration between all stakeholders engaged in different types of materials modelling, including modellers, software owners, translators and manufacturers;**

¹ open refers to the ability to combine different open source and proprietary elements, not to open source necessarily.

addresses the need to bring all stakeholders together so that complex industrial problems can be tackled successfully by drawing on multiple expertise. This will also enable identifying gaps in modelling and subsequently exerting collaborative efforts to cure them more efficiently than is possible today.

2. Facilitate integrated materials modelling in Europe building on strong and coherent foundations;

address a need to build, utilising this new collaboration, stronger foundations of modelling in Europe. This includes integrating material models with data repositories, data driven approaches (big data) and machine learning, integrated open simulation platforms and interoperability. Openness and interoperability will allow integrating open source and closed source commercial software and data equally which will lead to a boost in materials modelling due to more comprehensive exploitation of all available knowledge.

3. Coordinate and support actors and mechanisms that enable rapid transfer of materials modelling from academic innovation to the end users and potential beneficiaries in industry;

address a need to advance the translation and transfer process of innovation from academy to manufacturers. Improved transfer mechanisms will be stimulated to empower translators in academy, research organisations and R&D departments to harvest materials modelling foundations more diligently for the benefit of industry. This includes infrastructure such as Marketplace, which is a central hub for materials modelling in Europe, model validation repositories, enhanced training, and most importantly defining the role of Translators as specific stakeholders. There often a lack of awareness to the precise capabilities of modelling particularly in SMEs.

4. Achieve greater awareness and uptake of materials modelling in industry, in particular SMEs;

support actions in terms of workshops, case studies will be made to raise awareness, and consequently utilisation of materials modelling in all industry in Europe.

5. Elaborate Roadmaps that (i) identify major obstacles to widening the use of materials modelling in European industry and (ii) elaborate strategies to overcome them;

addresses future research needs that will stem directly from the actions of the EMMC. These will lead to more targeted research to close gaps in materials modelling and bring it up to the next level.

Taking all of the foundation and transfer elements together, the EMMC will be in a position to create impact in industry. The EMMC main objectives will be achieved via actions that make use of a range of accompanying measures, such as **workshop organisation** which bring together multiple stakeholders and target specific underpinning and enabling actions for wider adoption of materials modelling in industry. The actions will also include **targeted surveys** as a means to reach out for different stakeholders and gather rich information on a plethora of key topics.

3. EMMC Stakeholder Groups

The underpinning vision of the EMMC is that only when bringing all stakeholders together, sufficient synergies can be created to address the most challenging questions in materials modelling today and in the future. The key concept is to increase the interaction between all stakeholders to stimulate novel exploitation avenues of materials modelling based on collating expertise, models, knowledge and data. The materials modelling community consists of several stakeholders that are all represented in the EMMC:

Manufacturers: This group represents the interests of (current and future) end-users of materials modelling in small and large European manufacturing industry. It gathers key company representatives across industrial sectors, from consumer goods to industrial chemicals, from polymers to alloys etc. The objective of the manufactures in participating in the present project is to (i) clearly articulate commercial end-users needs, i.e. articulate what barriers need to be overcome to introduce materials modelling into their business cycle or enable an enhanced and more efficient/higher quality use of it, as well as what future developments they foresee to be necessary, (ii) provide case studies for the testing, validation and assessment of models, workflows, platforms and software. Actions will be taken in order to identify key areas of company interest for materials modelling solutions and how those can be achieved and act as a sounding board and participate in European consultation initiatives.

Translators: The successful application of materials modelling in industry depends heavily on translating industrial problems back into modelling questions, i.e. performing a process in the opposite direction to the value chain. Today, this role is performed by different actors, including R&D staff in large enterprises, application scientists in software companies, scientists in research institutions as well as individual consultants. The aim of the EMMC is to promote activities that optimize the roles of the translators by creating a set of open and transparent conditions and best practices as well as a resource of neutral competences available to all industry more widely, in particular to SMEs.

Software Owners: Software owners are defined as 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 freely as open source code, and proprietary software owners who sell their software to industry. A key objective of software owners is the transfer of materials modelling technology to end users, in particular manufacturing industry. One of the objectives is to identify where the current policies and programmes are supporting the industrial exploitation of academic and proprietary software, where there are gaps and where there are obstacles. The planned activities aim to provide guidelines on quality assurance in software development which aims to support the process of transferring academic software to the manufacturing industry.

Modellers: This stakeholder group consists of the developers of materials electronic, atomistic, mesoscopic and continuum models and respective solvers, as well as developers of coupling and linking schemes. The scope of this stakeholder group encompasses two main tracks of efforts: on the one hand, the stimulation of improved 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. Overall EMMC approach

The main overarching objective and goal of the EMMC is to allow European Industry to reap the benefits of materials modelling more effectively and vigorously. To this end, the EMMC has identified a number of core activities that are vital to increase the industrial exploitation of materials modelling in Europe. These activities can be structured into three main pillars on which the advancement of European Industry rests on as shown schematically in Fig. 2:

1. **Underpinning Foundations:** Stronger, more robust, better validated and more versatile materials modelling foundations. The existing **Foundations** in terms of discrete and continuum models, open simulation platforms, interoperability based on metadata schema will be further strengthened, and roadmaps established for future actions.
2. **Enabling Transfer Platform:** Designing the systems and mechanisms to transfer materials modelling to a range of industries. A **Transfer Platform** 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. These actions include a European Marketplace hub to ease the access of industry to materials modelling and data repositories, development of the Translators role and function, Training and validation of software.
3. **Integrated Materials Development:** Facilitating a more holistic materials development targeted at achieving tangible impact in different industrial applications. The ultimate goal is that materials modelling and simulation will become an integral part of product life cycle management in European industry, thereby making a strong contribution to enhance innovation and competitiveness on a global level.

Fig. 2. The three underpinning and enabling actions constituting the three pillars on which advancement of European Industry through advanced integrated materials modelling rests.

The main approach of the EMMC is to establish and enforce these actions by undertaking coordination and support actions for:

Model development and validation - aims at identifying model gaps, establishing Roadmaps to help cure these gaps and validate materials models as a joint activity between modellers, industrial stakeholders, translators and software owners.

Interoperability and integration - aims at providing operational infrastructures for interoperability of different codes and data of materials facilitating the integration of multiple models and tools to build integrated modelling workflows.

Modelling marketplace and data repositories - aims at promoting platforms providing ICT infrastructure for integration of materials models, development of workflows and access to concerted data repositories and collaboration platforms. It will engage in coordination and support actions to raise awareness for curation of materials data and will drive the proliferation of repositories. The Marketplace will also provide a central hub for materials modelling activities in Europe, including Training and Translation services for Manufacturers.

Translation and training from companies - aims at promoting and defining the role of Translators. EMMC will develop methodologies for Translators and translation processes adapted to various industrial sectors. Translators should be well knowledgeable with the capabilities of a wide range of materials modelling paradigms.

Industrial software deployment - aims at stimulating academic software exploitation, conformity to professional standards, user-friendliness and industrial exploitation. The goal is to enhance the level of software development, in particular in academy so as to enable more rapid transfer to industrial applications. Workshops on basic software writing will be recommended for new modellers as well as workshops on version control and testing suites. The EMMC will organize a white paper on software quality and software engineering advice. Furthermore, the activities will enable all stakeholders to optimise the process and the infrastructure which are necessary for the successful and sustainable industrial deployment of materials modelling software.

Industrial integration and economic impact - aims at assessing the economic impact of materials modelling on industrial prosperity, defining and documenting case studies (i.e. documenting successful as well as unsuccessful modelling cases in industry). The goal is to raise and measure the materials modelling impact with a specific emphasis on coordinating the development of Business Decision Support Systems (BDSS). These platforms should allow an end-user to select, connect and through multi-objective optimisation drive for options that make business decisions more data driven and acquire a higher level of efficiency for developing business cases as fitting into the industrial value chain.

From the current materials modelling state of the art the hurdles will be identified through industry consultation ensuring critical input to EMMC. It will ensure a feedback loop of continuous improved materials models and access facilities for advancing the ease of materials modelling implementation in industry. EMMC will bring together Modellers (discrete/continuum), Translators, and Manufacturers to tackle each activity in a collaborative manner, actively contributing to increase the interaction between all stakeholders. The interconnectivity and relations between these activities is shown schematically in Fig. 3.

Fig. 3. The interconnectivity and relations between different EMMC actions.

5. Impact of EMMC activities

The EMMC will enable industrial end-users to increase the quality and rate of innovation of their products by:

- Improved access to advanced materials modelling tools and databases.
- Enhance interaction and collaboration between all stakeholders.
- Better access to the large pool of knowledge of materials modelling which exists in Europe.
- Higher efficiency through integrated solutions of discrete and continuum models & materials databases.
- Clearly defined metrics by key performance indicators (KPI's).
- Clearer evidence of best practice in materials modelling.

The EMMC will achieve these as a result of:

1. Addressing (and providing roadmaps for) key issues in the underpinning foundations required to build a more integrated, open and accessible landscape, including the materials models themselves as well as their linking and coupling to support complex workflows, the interoperability and discoverability of models and data.
2. Facilitating an Enabling Transfer Platform consisting of human capital actions (Translators and Training), coordinated and more accessible knowledge sources and improved end-user software development and exploitation,
3. Supporting a more compelling business case for the application of materials modelling in industry via clearly specified, sector specific case studies, quality attributes, cost-benefit analysis and coordination and support for the integration of modelling into industrial decision support pathways.

a. Materials modelling and related databases will become much more accessible and usable.

Integration of communities, improved access and usability for a wider range of stakeholders entails agreeing on common nomenclature and metadata schema so that information can easily flow around and is categorised and searched in a unified manner. EMMC will pursue this goal by building on previous and ongoing actions such as the Review of Materials Modelling (RoMM) [2] and the Organisation of Modelling Data (MODA) and Metadata [3]. EMMC **will lead to greatly enhanced access and use of materials modelling** as a result of: (a) supporting the adoption of coherent terminology, which means that scientists that are not experts in modelling codes will find it much easier to understand and hence access what materials modelling does, (b) metadata schema that achieve a semantic level of interoperability, which means faster integration and easier access for people developing solutions, (c) de-facto standards for data structures and (d) modelling platform developments, which increase efficiency; EMMC will coordinate a reference design for Open Simulation Platforms supporting operation across different models, databases and the sub-disciplines of materials modelling. It means that codes can quickly be integrated, hence become more easily accessible and usable, (e) data repository design based on the above metadata schema which will facilitate translation and easier access to information across different fields, and (d) establishment of an ICT platform to manage the materials modelling knowledge and information in Europe, including new sustainable collaboration channels that break through current community barriers. By means of the above actions, EMMC addresses the obstacle that “the interoperability of software and data is a major barrier resulting in limited use of (integrated) simulation software by non-simulation experts”[4]. It will lead to reducing the efforts required for designing advanced integrated workflows impacting therefore the utilisation of materials modelling in industry. In addition, the increased use of databases will allow novel routes to develop new materials with specific properties harvesting existing and future materials data.

b. Better access to the large pool of knowledge of materials modelling which exists in Europe.

Industry requires a one-stop-shop, a gateway to all materials modelling relevant information. This includes in the first instance materials data linked to Models and Software Solutions used to generate the data, validation information on the models and verification of software solutions. Such information allows stakeholders a complete view of the relevance and quality of a particular data element and its applicability in a specific workflow. Added to that will be human resources by linking of data and models to respective Modellers (both creators and general experts) and relevant Translators, allowing Manufacturers direct, more targeted interaction with Modellers and Translators. Finally, this information is augmented with additional documentation resources such as show-cases, education and training, case-studies and linked publication repositories. EMMC will coordinate and network with relevant stakeholders, technology platforms, excellence centres and projects to work towards the design and establishment of a European Materials Marketplace as an open Gateway connecting for information and knowledge management in materials modelling. This will support federated resources of materials data and information repositories, curation of data and information, active collaboration between stakeholders, computational modelling services and education and training. This will impact material modelling in Europe on all levels, in particular enhancing the Human Capital factor by empowering all stakeholders and bringing them together regardless of geographical or community barriers. It will impact the proliferation of knowledge source and material data repositories, speed of publication and dissemination as well as increased novel collaboration channels.

c. Higher efficiency through integrated solutions of discrete and continuum models & materials databases for industrial use.

As mentioned in a TMS study [5], successful execution of a project in industry depends upon a broad range of tools and methodologies that must be reliable, cost effective, verified and validated to ensure the accuracy of the results. EMMC will coordinate the definition and acceptance of standards for metadata and simulation platforms supporting the efficient integration of modelling components for different length- and time-scales into comprehensive modelling systems. It will build on foundations laid by the EMMC and the European Multiscale Materials Modelling cluster and ensure that an interoperability level is agreed on, which would form the basis for implementations across all levels of materials modelling as well as materials data. The Roadmap of Materials Models will identify opportunities and gaps for coupling and linking of models. It will be an essential compendium of methods and spawn more targeted research. Within the EMMC, interactions between industrial end-users and the EMMC partners will identify and focus on areas where urgent and highly relevant industrial problems can be addressed with materials modelling of the most mature technology readiness level. In other words, the EMMC will at first emphasise application areas, which have the highest and most immediate industrial and societal impact.

d. Increased efficiency and industrial effectiveness of materials models in industry and research.

Many industrially urgent and unsolved problems can be tackled with today's materials modelling capabilities provided that these problems can be translated into modelling strategies leading to tangible result. The EMMC will support the development of the role Translators, who play a critical role in achieving a higher and faster impact of materials modelling. EMMC will support the development of methodologies for Translators, translation processes specific to different industry sectors, and implementation of methodologies for using model workflows, including identification of software components connecting models operating on different scales. A strengthened, more widely available and trustworthy Translator function will enable industry to decide on where and how best to use modelling to greatest effect. Training courses with a focus on how to use the progress in materials modelling and simulation in order to support industrial innovation will contribute to increased efficiency and industrial effectiveness. Training will also increase the awareness in industry about modelling software and data resources available. Furthermore, modelling experts and translators will become more efficient and effective as a result of EMMC interoperability actions as they will be able to choose and utilise models much more efficiently. Further actions of the EMMC that impact efficiency and industrial effectiveness include improved quality and end-user ready (commercial or open) software, easier access to information and knowledge via metadata and marketplace, best practice cases, know-how about what works and what doesn't and hence focus on relevant key performance indicators.

e. Establishment of technical and business-related quality attributes (Key Performance Indicators) that inspire trust in materials modelling.

The use of modelling in industry today is hindered by a relatively low 'level of acceptance' which is often due to the difficulty to appreciate what modelling actually can and cannot bring and how exactly it will affect the commercial offering of differentiated products. Consequently, the uncertainty and risk for a major engagement (i.e. investment) in materials modelling is often unclear. This is compounded as no single model or software exists to address all the critical (often conflicting) performance criteria and various options that define a differentiated product offering. EMMC will counter this and create impact by compiling a catalogue of case studies to provide tangible facts demonstrating the impact of materials modelling in particular applications. The EMMC will consider the business case for modelling by spawning a cost-benefit analysis and demonstrate the value of materials modelling by using suitable technical and business related KPIs. This work will build on the survey and report [1] on the economic impact of materials modelling which identified already a range of KPI categories. EMMC will also work closely with the forthcoming BDSS projects and EMMC supported Translators in the definition of technical KPI models as functional of the materials modelling state variables, and coordinate the way in which the technical aspects of an industrial problem are mapped to a multiscale modelling workflow, and represented as a KPI model. The Translator will support the end-user in deciding business oriented quality attributes, which may depend on the modelling state variables as well as for instance costs, and processing time, which usually depend on the material variant currently simulated in the modelling workflow. The role of EMMC in inspiring trust will be to support, coordinate and disseminate demonstration examples of implementation of KPI driven workflows in industrial applications. Also, a training guide for industrial operators using these methodologies will be developed. Further EMMC actions that will contribute to a greater level of trust include laying out clearly the current strengths and current gaps in the Roadmap, a best-practice guide for standardizing the error estimates of materials models, and model validation guidelines.

f. Industrial best practice (methodologies) for end-users increasing speed of development in industries

The EMMC will support best practice by a range of actions. Methodology development on Use Cases defined together with manufacturing industry organisations will be carried out by Translators who will define best practice in specific industry applications. The actions on Training support workforce development regarding skills required to launch effective materials modelling supported programmes and will increase the confidence, speed and success of implementation and hence development in industry. The EMMC will work with stakeholders to define the

expectations of a materials modelling function in an organisation more clearly (the What, When and How) and define measurable impact levels that this function can be appraised by. Experience from Computer Aided Drug Discovery shows the benefits of this process in terms of trust as well as performance [6]. Working Groups will be formed and Workshops organised to discuss and endorse recommendations and guidelines for best practice. Practitioners will be supported to include a careful economic analysis of the cost and savings associated with implementing materials modelling. EMMC will gather requirements and coordinate the planned Business Decision Support projects to provide both best practice guidelines and a coordinated platform for an economic analysis.

6. Conclusion

EMMC will undertake the actions in order to close the gap between materials modelling and manufacturing. It will aspire to eliminate or at least significantly contribute to substantially reduce the innovation valley of death by strengthening and incorporating the underpinning and enabling actions into the modelling landscape in Europe. The definition of the role of Translators, the development of data repositories based on standards and interoperability, increased collaboration between all Stakeholders and validation actions are all only but one part of the whole picture.

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