The European Materials Modeling Council

The EMMC Roadmap 2016 for Materials Modelling

The EMMC is proposing underpinning and enabling actions that will increase the industrial exploitation of materials modelling in Europe. This document presents the needs of a large set of players in the materials modelling field. The EMMC requests the EC to recognize the topics identified as topics of Europe-wide interest. The activities proposed need to be developed to TRL7 which would fit with the scope of the LEIT programme. The implementation (TRL 8-9) will be up to the individual organisation/academic or company and can become a proprietary exercise. This phase where results can then be customised and used in commercial operations is not addressed in this Roadmap. This Roadmap 2016 represents an extension of the previous Roadmap 2015.

Summary

The Roadmap recognises the importance of making advances in materials modelling to support the competitiveness of European industry. It strives to identify gaps and actions to address them based on a rich input from and discussion between the different stakeholder communities organised in the European Materials Modelling Council (EMMC). More systematic inputs were collected by a dedicated online survey, which was sent to more than 1500 stakeholders. The stakeholders cover the whole spectrum of the Material Modelling Community in Europe: industrial end-users (manufacturers); software owners; translators and modellers. Often one organisation plays more than one of these roles. The wide European stakeholder consultations conducted within EMMC proposes that the EU LEIT Work Programme 2018-2020 should be used

- ***To promote materials modelling as a key enabling technology for the Digital Single Market (DSM):** Predictive multi-scale modelling has the potential to become an integral part of value chains providing economic advantages for all manufacturing industries, by enabling new solutions and supporting technology transfer. Activities will focus on meeting the modelling needs of industrial end-users, accompanied by relevant translator services, metrology, instrumentation, standardisation as well as support tools for business decision;*
- ***To promote materials modelling for science-based risk assessment and regulatory aspects**: In the case of nanomaterials, the fast evolution of the market is not matched by equal progress in the regulatory framework, resulting in the lack of regulatory clarity. This hampers the uptake and exploitation of products and materials involving nanotechnologies and may become a major barrier to innovation. A safe and sustainable development of nanotechnology products is needed both for public protection and for innovation to meet societal needs. This is expected to be an important market enabler for the European*

manufacturing industry. Besides accurate quantification of the eventual risk in regulatory terms, advances in this area may also deliver safety-by-design protocols and methods that would bring management of this risk to equal levels as for other known risks.

More specifically, these are the topic areas which require urgent actions.

Materials modelling as key enabling technology for the Digital Single Market (DSM):

1. *Translation*
    a. *Topic 1a: Accelerating the uptake of materials modelling in European Industries by establishing an intermediary translation process*
    b. *Topic 1b. Enhanced innovative industry-modeller intermediary network for increased uptake of materials modelling in European Industries*
2. *Business integration*
    a. *Topic 2a: Reliable top-down and bottom up design of new materials and processes by coupled/linked models for faster products development*
    b. *Upscaling of European strongholds in materials modelling*
3. *Upscaling of European strongholds in materials modelling*
    a. *Topic 3a: Accelerated upscaling of European strongholds in materials modelling into commercialised/market solutions*
4. *Market Place*
    a. *Topic 4a: Advanced platform for integrated materials modelling and product development to support EU business environments on the EU Marketplace*
    b. *Topic 4b: Innovative system for the integration of current material modelling / Standardised Platforms to integrate existing materials models to solve complex industrial workflows*

***Materials modelling for science-based risk assessment and regulatory aspects**:*

5. *Materials Safety, Efficiency and Risk Assessment*
    a. *Topic 5a: Physics/chemistry-based materials modelling in assessing nanotoxicity for health and medicine*
6. *Characterisation and Modelling Integration for improved production and upscaling.*
    a. *Topic 6a: System for the integration of measured and simulated data into production value chain*
    b. *Topic 6b: Integration of materials modelling into production and quality control*
    c. *Topic 6c: New design modelling for improved reliability and sustainability of microstructured materials*

***Coordinating network**:*

7. *Coordination and Support*
    a. *Topic 7a: A network to capitalise on the strong position of materials modelling in Europe and accelerate the transfer of academic knowledge to industrial applications*

Contents

1 Introduction

This Roadmap is elaborated by the European Materials Modelling Council (EMMC). The EMMC has the goal to be aware of and network (loosely or strongly) all major existing activities in the field of materials modelling in Europe. The aim of the Council is also to establish current and forward looking complementary activities necessary to bring the field of material modelling closer to the demands of manufacturers (both small and large enterprises) in Europe.

How was the Roadmap elaborated and endorsed?

Since 2014, EMMC has worked towards defining the most relevant and urgent actions needed in order to promote the use of materials modelling in the industrial sector. We have felt the need to systematically consult a large set of stakeholders and hence designed an online survey about materials modelling needs. More than 1500 stakeholders were invited to fill in this survey and we elaborated the feedback from more than 250 participants (20% are manufacturing industries and 40% software owners). The survey largely confirmed the most critical actions identified by the EMMC, but it also provided new ideas which have been used as a basis for this Roadmap. We asked each participant to rank each topic in the range 1-5 (1 being the most important), in terms of importance and urgency of the topic. We assumed the score 6 when no reply was provided for a specific topic. In the following table, the topics are reported in the decreasing order with regards to the product of importance and urgency, used as in indicator of the relevance of the action, namely Relevance = Importance x Urgency.

Topic	Importance (1 = highest)	Urgency (1 = highest)	Importance*Urgency
Coupling/Linking	2,13	2,19	4,67
Discrete models	2,21	2,35	5,18
Properties	2,25	2,45	5,51
Industry 2020	2,45	2,55	6,25
Accuracy	2,52	2,63	6,62
CSA	2,74	2,80	7,68
IntOp	2,74	2,81	7,71
MMP	3,15	3,21	10,10
BDSS	3,14	3,26	10,26

The full analysis is documented in a report which is publicly available on the EMMC web site. The results of the survey were presented and discussed during an EMMC Roadmap meeting in Brussels on 20th May 2016. The 10 topics reported in the survey were put online in the collaborative wiki for further discussion in June and more comments were collected. During the summer 2016, these 10 topics were elaborated again and better group in the current 7 categories with proper sub-topics (see above in the summary and next for further details).

2 Objectives and Vision

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 enhanced innovation and competitiveness on a global level.

The impact of materials modelling on the industrial sector relates to a number of aspects:

- The increased cost of developing a 21st century product, with all its specifications, requires a clever and targeted design procedure where a performance-based (back-engineering) functionality of the product is guaranteed. Here materials modelling is an essential component.
- Virtual integration of processes will reduce costs.
- Materials modelling is already part of many business processes but can become a more crucial part if the economic advantage for the end-user is made clearer.
- The majority of managers (in SMEs) are not aware of the importance of proper modelling-assisted materials selection and sourcing procedures and the improvements that can be achieved with respect to quality and functionality on one side and the costs on the other. Increased awareness of the modelling potential here, as well as of training opportunities and the availability of a materials modelling market place, will be important.
- Materials modelling can help minimize expenses and time needed in achieving a functional and marketable end product.
- Interesting vision: availability of proper models for any given manufacturing problem; this would be a strong asset. For example, additive layer manufacturing is an area where materials modelling are essential, but where the physics of the phenomena is poorly understood. Thus modelling through many length and time scales, and throughout the production process itself, would be very valuable.
- It is crucial to increase modelling impact in the framework of Industry 4.0, and to develop process-to-end-user (material performance) workflows and toolsets.
- Virtual factory models would revolutionise manufacturing. This requires levels of IT expertise much beyond that of traditional modellers; partnerships are vital here for the upscaling of materials models to include databases towards development of business decision making software tools.
- Materials discovery. The use of theoretical models and workflows to propose novel or modified functional materials and motivate further experimental work is already now becoming a reality, but the impact of such activities on the final business value is likely to require a longer timeframe (> 10-15 years). Here, an appropriately and thoroughly designed Roadmap towards theoretical discovery of new materials will assist to accelerate the implementation of new and better materials. To this end, efforts on the development of new structural search engines, structure-properties descriptor analysis tools, efficient workflow schemes, and improved and widened discrete models are needed at this stage.
- Reducing the variance of a chemical product is yet another important area where modelling will be of practical importance, e.g. in the analysis of the origin of such variance.

In recent years, materials modelling of nano-scale phenomena, especially that based on discrete models (electronic/atomistic/mesoscopic) has developed rapidly. However, this has not yet led to the integration of these models as part of the industrial design tool chain of materials and products. The European manufacturing industry requires faster, more reliable modelling of novel advanced nanomaterials and technologies and of new applications of existing materials. Furthermore, it desires linkable tools that allow closed loop optimisations combining the simulation of manufacturing process on all scales, component design and quality assurance. The main goal of the EMMC is therefore to stimulate the industrial exploitation of discrete and continuum modelling approaches applied to material phenomena occurring at the nanoscale in industry by linking them to the already well-established continuum-models applied to the macroscopic (device) scale. To achieve this challenging objective, the EMMC has so far identified a number of core activities that expand the ambitions concerning better, more accurate and realistic discrete or linked models, but also reaches out to other crucial elements such as how to further promote the Digital Single Market (DSM) and how to develop science-based risk assessment and regulatory aspects.

The vision of the EMMC is that only by considering all these elements together sufficient synergies can be created that will allow Europe to address the most challenging questions in materials modelling. One of the central visions of the EMMC is to enable manufacturers to utilise modelling in their business decision support cycle, much as this is done today with experiments. The aim is to bring material modelling one step closer to manufacturers and to better integrate materials modelling into industrial processes. Many challenges lie along the road towards this goal, and some of the most important ones are addressed in this Roadmap. It will be updated regularly as new challenges arise.

This Roadmap shares many ideas with a recent book, titled **Open innovation, Open science, Open to the world – a vision for Europe** [doi:10.2777/061652]), from the Directorate-General for Research and Innovation. These three concepts of openness are fully consistent with the visions of the EMMC, which is a bottom-up organisations that promotes the involvement of all different types of stakeholders in the modelling eco-system and, furthermore, places *the users* in the spotlight, in line with the ideas expressed in the mentioned document. Also in line with the vision of The Three Os, the EMMC supports the idea of allowing users to share a common platform to exchange knowledge; its creation is on the EMMC agenda. Furthermore, the EMMC is very open to the world and to international collaboration, as demonstrated, for example, by the formation of the International Materials Modelling Board (IM2B) as a framework for the Council's international involvement.

3 Where are we today?

Towards materials modelling as key enabling technology for Digital Single Market (DSM)

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, large and small companies rely on numerical simulations to effectively and efficiently design and engineer new products and thus minimise 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 cost of manufacturability 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, 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.

While applications to both materials and manufacturing process design have been demonstrated, **modelling today is not always the essential tool in commercial development** because **modelling tools are often seen as difficult to use**, **not accurate enough**, or unable to deliver **answers to very specific questions**. There remain a number **of technical challenges to develop novel models that are *both* reasonably easy and affordable enough to use *and* predictive (i.e. accurate enough)** to enable the desired novel product design.

Numerical simulation in industry **today** is mostly dominated by Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) solved by Finite Element or Finite Volume Analysis, and these continuum models form part of the Product Lifecycle Management/Computer Aided Engineering (PLM/CAE) process. 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. The continuum models for products and processes need to be linked to discrete and continuum models applied to finer scales to give accurate results on larger scale and to achieve sufficient resolution where it matters. More and more companies have recently started using discrete (electronic/atomistic/mesoscopic) materials modelling to include more detail in their simulations. With the increasing importance of materials for the European competitiveness and sustainability, it is urgent today to **develop the materials modelling community, to mature the tools for an effective and efficient use across various industry sectors and application areas and to facilitate industrial exploitation, in order to make materials modelling a key enabling technology for Digital Single Market (DSM)**.

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. A common weakness in today's software lifetime is the discontinuity that might take place when the initial developers (e.g., Ph.D. students, post-docs, etc.) leave the development team, or when the software moves from academia to commercial software owners. Another issue in software exploitation today, which can be a bottleneck when transferring or using software from academia to industry, is the software licensing scheme, which in many cases is too restrictive.

Another challenge concerns the fact that much development in modelling and its application in industry is hindered by lack of communication and interaction, on the one hand between modelling communities who may in fact struggle with similar obstacles and where synergistic progress would speed-up and improve the development process, and, on the other hand, between different stakeholders. Im either case, lack of construcive communication, leads to severe waste of resources and, in the end, a more limited use of modelling by manufacturers. The communication modes and patternsneed to be increased and improved and new avenue to connect the stakeholders need to be explored.

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 are many good examples of important and impactful topics that can be addressed with already existing materials modelling technology. However, there is generally a lack of dissemination and translation of such knowledge into industrial applications. Likewise, there is also a lack of information transfer concerning approaches which do NOT work, which is an important enouh aspect.

In manufacturing companies, modelling typically resides purely within the realms of R&D departments and materials modelling is not yet used in daily operations. Materials modelling today is often focussed on characterisation and understanding of physical phenomena, an activity which is clearly very important but not sufficient for integration of modelling into engineering design and business decision processes and systems.

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 "end-users", 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 would be required. In other words, acceptance and adoption of modelling material properties instead of experimentally measuring them for certification and validation purposes must be enhanced.

There is therefore a need to establish a trusted process to incorporate 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, today, allow fast and reliable simulations of many material properties and systems thus allowing modelling of a large variety of technological processes. The number of key players and stakeholders engaged in various modelling activities, including electronic, atomistic, mesoscopic and continuum models (e/a/m/c) in Europe islarge. The explosion in the number of models (and the data related to models) makes it **difficult to find the most relevant solutions in a timely manner** and it is often unclear or intricate which models , and which software tools, that are available and appropriate for a particular physics/chemistry problem. *There is currently no common platform that manages the materials data and knowledge infrastructure.* 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 [3]. It is very difficult 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 will present 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 modelling data and knowledge in a well-structured and standard form.

There are substantial barriers in the way to integrating materials models and databases into business decision support systems. Materials models lack the level of accuracy, robustness and good uncertainty 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.

Successfully addressing these challenges will allow 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.

Towards materials modelling for science-based risk assessment and regulatory aspects

Nanomaterials (NM) are produced in a high number of versions due to variations in chemical composition, size, shape as well as by employing different chemical surface modifications. Thousands of new nanomaterials are entering the market annually. Thus, the current number of NM variants is enormous and even more are in the pipeline in R&D. For each NM variant plenty of material characterization data are needed, which are often referred to as intrinsic NM properties. However, during the life cycle the NM change their properties in particular when they come into contact with biological matrices or the environment. Therefore a similar number of system-dependent properties, also referred to as extrinsic properties, have to be assessed as well. Most of these properties influence the fate and the effects of NM in cells or tissues.

Modelling nanotoxicity is about predicting the risk due to the use of NM. Risk is defined as the probability that exposure to a hazard will lead to a negative consequence for the cell fate, or more simply, Risk = Hazard x Exposure. Hence modelling nanotoxicity is based on two types of models:

- Exposure models;
- Hazard models.

Exposure models are intended to predict how NM evolve in the environment, including aggregation, and hence may harm human health and/or wildlife. On the other hand, hazard models are intended to predict what happens when NM come in contact with living cells and tissues. Hazard models can be split into three different steps:

1. Modelling how electronic and atomic properties, namely physics and chemistry, determine the nano-descriptors, which summarize the most relevant information about NM (materials modelling);
2. Modelling how nano-descriptors are correlated with most significant biological endpoints, namely those specific biological events which are supposed to drive adverse events (biological event modelling);

3. Modelling how one or more endpoints are significant markers of adverse events for living cells in contact with NM (computational systems biology).

4 Stakeholders

4.1 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 this stakeholder group is to clearly articulate commercial end-users needs to introduce materials modelling into their business cycle. 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.

4.2 Translators

The group of Translators within the EMMC consists of people, experienced in “translation”, from industry, research institutes and universities. Although these Translators have a working knowledge of how to approach industrial challenges by materials modelling, they feel the necessity to develop a self-contained role description of Translators around technical quality attributes, commonly called Key Performance Indicators (KPI), obtained by modelling. However, in an industrial context business related measures like pricing, time to market and sometimes even regulatory issues are usually as important as the KPI's. This aspect of “translation” is usually not taken into account today and this is one reason why industry is currently not fully unlocking the potentials of modelling. Translators within the EMMC will take these business oriented measures into account from the very beginning to the benefit of manufacturers.

The Translator role is not meant to replace or overlap with existing efforts, but rather to significantly extend them and enhance their functioning by providing a more complete and wider expertise across the EMMC.

4.3 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 models to end users, in particular in manufacturing industry.

The Software Owners group will identify where the current policies and programmes are supporting the academic and proprietary software owners and where there are gaps. The group has already established guidance on quality assurance in software development which aims to support the process of transferring academic software to the manufacturing industry. This document can be found on www.emmc.info. Licensing policies, standards and software documentation are discussed and recommendations made.

4.4 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. As such the stakeholders are organised in sub-groups representing these various aspects.

The scope of the stakeholder groups 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.

4.5 Council: stakeholder organisation

There is a need for an overarching organisation that will build up the constituency and networking the relevant stakeholders. The materials modelling community consists of many stakeholders (manufacturers/end-users, electronic/atomistic/mesoscopic/continuum), open source/proprietary software owners, service providers/translators etc.). There is a need for increased interaction between these stakeholders so that they can stimulate exploitation of materials modelling and can establish Roadmaps to guide the necessary developments in the field.

5 Key topics needing action

In order to exploit the academic materials models that exist there should be a focus on successful transfer to the industry of the enormous potential. The EMMC identified **seven key topics** (and their subtopics) that need attention at this moment:

5.1 Translation

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. In fact, no industrial project using materials modelling could ever be launched without some translation effort. Today, this 'Translator function' 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. However, while the role as such already exists to some extent, there is no wide-spread recognition of the Translator as a key actor with a well-defined role. One value in establishing Translators as recognised actors in the process lies in 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.

Action(s):

5.1.1 Topic 1a: Accelerating the uptake of materials modelling in European Industries by establishing an intermediary translation process

Outcome:

- An intermediary process/system that translates an end user specific problem to a modelling workflow
- an open translation environment for the optimisation and development of novel materials and products to link materials modellers with translators and end –user industry through the integration of modelling into one coherent and seamless system.

Impact:

- Increased speed of material/and or product development time
- Drastically reduced development costs for industry
- Rapid design from concept to market
- Increase the knowledge-base of European industry
- Allow reuse of materials modelling knowledge and expertise in different industrial domains
- Cross-industry fertilisation by use of the protocols and systems in other relevant areas or sectors beyond the ones covered by the project.
- Increased use of materials modelling in industry

5.1.2 Topic 1b. Enhanced innovative industry-modeller intermediary network for increased uptake of materials modelling in European Industries

Outcome:

- Install a network of modelling hubs in Europe. Facilitate the exchange of non-competitive "know-how" in modelling technologies which will benefit the innovative potential of diverse industrial sectors, relevant in both SMEs and in large corporations:

Impact:

- Increased innovation in industry based on materials modelling
- A strengthened European materials industry in a highly competitive market
- Increasing awareness of designers about new materials
- Awareness of industry in general and SMEs in particular of the rapid progress of computational materials modelling tools, and increased use of materials modelling by the manufacturing companies (end-users);
- Broad, fast, and easy information management and exchange between the modelling community and industry
- Rational development of sustainable developed products and processes;

5.2 Business integration

The use of materials modelling in industry models in decision making requests that models provide results validated in the operational practice. These models need to be integrated with business decision approaches to enhance effective decision making.

BDSS is one of the key needs of the industrial and manufacturing process. It should address key challenges such as how to connect across different business units and different functions to make better decisions with known cost implications. The business case for this is clear: it implies essential savings in time and money, especially if it can eliminate the need for (some) plant trials.

Action(s):

5.2.1 Topic 2a: Reliable top-down and bottom up design of new materials and processes by coupled/linked models for faster products development

Impact:

- Provide additional exploitation channels for academics
- Use of protocols, workflows and workbenches in other relevant areas or sectors beyond the project
- Predictable and trackable simulation workflows
- Growth of commercial SWO companies
- Contribute to boosting jobs and growth of investment of software owners in Europe and strengthen their international market position
- Inclusion of discrete models into a coherent materials modelling platform, as part of the DSM
- Digitalization of data gathering and the associated procedures to determine accuracy and precision of datasets.
- Digitalization of procedures and methodologies integrated with calculations routines facilitates experimentation, reduces error and enhances efficiency of the operation.

5.3 Upscaling of European strongholds in materials modelling

In manufacturing companies modelling typically resides purely within the realms of R&D departments and materials modelling is not yet used in daily operations. Materials modelling today is still largely focussed on understanding of physical phenomena. While the importance of this should not be diminished, it is not sufficient for integration into engineering design and business decision processes and systems.

Action(s):

5.3.1 Topic 3a: Accelerated upscaling of European strongholds in materials modelling into commercialised/market solutions

Outcome:

- Provide industry-ready integrated, standardized, interoperable software solutions starting from academic software or knowledge results from existing and past projects.

Impact:

- Provides additional exploitation channels for academics and research organisations in Europe
- Growth of commercial SWO companies
- Increased upscaling of software solutions in Europe
- Contribute to boosting jobs and growth of investment of software owners in Europe and strengthen their international market position
- Reduce costs of development of new products and solutions for the European Market
- Contribute to reduction of costs of upscaling and securing markets for European industries, especially SME software owners.
- Increased use of discrete models in industry
- Better sustainability of developed materials models
- Better, faster, optimised materials modelling suites

5.4 Market Place

There is a need for a Materials Modelling Hub, a platform for the information exchange on key issues concerning materials modelling and its industrial application. This platform should enable exploring possibilities of materials modelling approaches and should offer novel solutions to the entire European material modelling community. 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 links between the areas of fundamental material modelling and their potential applicants (beneficiaries) represent at present one of the major obstacles for further progress of material science. There is therefore an **overarching need for the development of a system that integrates the materials modelling components**. A Modelling Market Place containing databases and libraries of models and data, validation information, educational resources, model selectors, benchmarking possibilities and advice for workflows will fill this need. Such a system will assist and further strengthen R&D foundations in Europe ensuring its continued leadership in advanced technology and modelling.

Action(s):

5.4.1 Topic 4a: Advanced platform for integrated materials modelling and product development to support EU business environments on the EU Marketplace

Outcome:

- A suite of integrated and interoperable materials modelling apps that combine databases of models and materials properties along with expertise exchange and translation services to support existing and future European Materials Modelling Marketplace hubs. In particular the development of apps that can be integrated readily in Business support systems to assist rapid and efficient decision making is expected.

Impact:

- Better integration of materials modelling in the industrial process
- Bring materials modelling to the heart of industrial business decision making levels
- Allow industry and translators to rapidly build custom designed integrated materials modelling apps and data driven business decision systems
- Reduce the costs and time to market of novel materials and products
- Allow reusability of the developed apps in multiple application fields
- Increase the knowledge base of European industry and allow new avenues for upscaling of materials modelling tools through exploitation by software owners on the Marketplace hubs
- Contribute towards a coherent DSM in the field of materials modelling
- Broad, fast, and easy information management and exchange both between the modelling community and industry and within the modelling community;
- Improved decision making on the level of materials and sustainable market differentiating products
- Allow industry to react to changing market and regulatory demands
- Reduce the need to at least some field tests

- Enhance the ability for manufacturing companies (end-users) to do an effective search of numerical tools and/or providers of numerical simulations who could best suit their needs and to build required workflows without expert knowledge in materials modelling
- Supply of software developers with comprehensive information about the potential clients and industrial tasks where numerical simulations would be highly desirable;
- Rapid deployment of novel materials modelling solutions in particular in manufacturing-targeted domains.
- Developing alternatives for more sustainable product development that reduce the overall environmental footprint.
- Develop functional and responsive materials that combine several features performance into one material in particular for responding to different environments of use and lifecycle stages.

5.4.2 Topic 4b: Innovative system for the integration of current material modelling / Standardised Platforms to integrate existing materials models to solve complex industrial workflows

Outcome:

- The modelling framework should allow the seamless and standardised integration of various existing models, based on existing and emerging standards for semantic interoperability across domains

Impact:

- Speeding up the rate of industrial transformation to high-added-value products
- Improved decision making in process development and testing.
- Accelerated introduction of new materials and/or manufacturing parameters.
- Development of better manufacturing technology.
- Improved, faster and cheaper evaluation of production process deviations without the necessity of destructive testing.
- Faster and more assured introduction of the manufacturing process.

5.5 Materials Safety, Efficiency and Risk Assessment

Development of nanotechnologies and nanomaterials, on the one hand, provides us with new opportunities for diagnosing or treating many of the remaining intractable disease classes (viral, genetic, cancer) using nanoscale agents or tools, which can be tailored to deliver precisely targeted action. The use of nanomaterials thus forms a technological core of personalized healthcare, which is expected to be one of the biggest paradigm-shifts in medicine. Predicting the impact of different dose schedules on healthy and diseased bodies, cross-interactions among different drugs and planning for administering drugs will be essential in the future therapies. With this regards, materials modelling may provide the right connection between drug design (already done in some cases by materials modelling, at least as preliminary screening) and biological events. This goal is extremely challenging because the interaction of drugs with each other and with the functioning of an organism is extremely complex, and predicting this interaction goes well beyond the approach relying on nano-descriptors. One would need to quantify specific drug-protein and drug-nanocarrier interactions and then integrate them into a computational systems biology approach to build a reliable model.

On the other hand, the use of nanomaterials presents a variety of unforeseen risks, as the nanoparticles challenge the immune system of the human body at lengthscales where it is not well prepared to react. Even some of the nanomedical systems have demonstrated unforeseen toxic properties. The understanding of the mechanisms of potential nanomaterial-induced hazards would enable manufacturers to quickly screen out particles with physicochemical properties related with a risk, and either develop new particles or re-engineer their products to modify their properties to exclude the risk factors, and provide nanomaterials which are safe-by-design. The risks should be defined in a broader sense to include any adverse outcome induced by an exposure to nanomaterials, which requires integration of the materials modelling with systems biology.

A development of a joined approach is therefore necessary, where nanomedicine and nanosafety will rely on the same body of knowledge, based on the understanding of the interactions between nanoscale objects and living systems, i.e. bionano interface, and its relationship with systemic responses. Materials modelling is currently in a strong position to support this development by addressing physicochemical properties of bionano interface at a systematic quantitative level.

Beside the nanosafety and nanomedicine, accurate modelling of bionano interactions has a potential to benefit other industries related to health and wellbeing. Materials modelling can contribute to assessing materials toxicity in order to reduce animal experiments in cosmetics and personal hygiene products. It can also provide a boost on understanding the processes of degradation in food, e.g. related to fouling, and on assessing the toxicity of food after exposure to different contaminants, as well as on improving food processing technologies, where organic-inorganic interface are involved. The overall economic benefits for EU industry from the use of materials modelling can be foreseen in the field of nanomaterials production through support of development of materials that are safe-by-design, reduction of administrative burden related to toxicity assessment, and improvement of time to market especially for SMEs dealing with nanotechnologies. In addition, the understanding of the toxicity mechanisms will help to improve public acceptance of nanotechnologies.

Action(s):

5.5.1 Topic 5a: Physics/chemistry-based materials modelling in assessing nanotoxicity for health and medicine

Outcome:

- Physics/chemistry-based materials modelling will improve the predictive power of exposure models and enable mechanistic models of hazard by providing a quantitative description of NM aggregation in different environments – including self-aggregation, NM dissolution, NM reactivity and binding to biological macromolecules in a biological milieu (e.g., formation of a protein corona, adsorption to and penetration through membranes), and interaction with natural organic matter in soil and natural waters. From the perspective of environmental fate and transport, materials models must provide reliable input information (e.g., aggregation/agglomeration/dissolution, sedimentation, solubility, partition coefficients, reactivity) for multi-media modelling.

Impact:

- Ensuring the safety of all newly produced NMs. The integration of material models with exposure and hazard models will facilitate the development of safe NMs by including nanosafety constraints in its computational design. More specifically, a progress in modelling NMs and bio-nano interactions will facilitate faster definition of NM toxicity mechanisms, hazards and risks. Knowledge of the mechanism of action of each NM will enable identification of biomarkers for exposure and health effects.

- Opening new ways for diagnostic and treatment of disease. Predicting the impact of different dose schedules on healthy and diseased bodies, cross-interactions among different drugs and nanocarriers and planning for administering drugs will be essential. In this respect, materials modelling may provide the right connection between nanodrug design (already done in some cases by materials modelling, at least as preliminary screening) and biological events. Material models can contribute to link structural and physicochemical features of nanoparticles with their diagnostic use and therapeutic effects (e.g., maximizing the killing of damaged cells while minimizing the effect on healthy cells).
- Reducing significantly (and ultimately avoid) animal experiments. Estimates for the needs of animals for in vivo testing exceed what is considered reasonable in any modern society, where particular emphasis is given towards the need to reduce reliance on animal models.
- Clarifying organic-inorganic interactions. The methodology for modelling bio-nano interactions will have wide implications in other fields, such as food science, pharmaceutics, and medicine, where organic-inorganic interactions are important.
- Improving life-cycle analysis of all nano-enabled technologies. Whilst in no way diluting the importance of nanosafety issues of consumer-oriented products, there is quite clearly a longer-term aspect of science to be addressed. Thus, the key issues of where nanoparticles go, and their interaction with living matter is a long-term question, which will have implications for life-cycle analysis of all nano-enabled technologies, including those never intended for contact with living systems.

5.6 Characterisation and Modelling Integration for improved production and upscaling

Industry requires validated material model workflows and validation is requested of the models in an industrial context, as the context defines the quality attributes of the solution. These quality attributes should include technical as well as business (like time to solution and money to be invested) aspects as all those quality attributes are an integral part of a Business Decision Support System. Linked to the validation question are benchmarks for data and applications, in depth success stories but also more room for public discussion about approaches which do NOT work. The latter is poised to be a lever to identify deficiencies of existing models, and hence ignite future concerted research activities and efforts aimed to enhance existing models.

A facility to develop and coordinate the necessary characterisation and validation methodologies is needed.

Each of these key- and subtopics will now be discussed in separate chapters, where the objectives and the requirements that must be met and the actions that are needed in order to realise the objectives for detailed topics supporting the objectives will be outlined.

Action(s):

5.6.1 Topic 6a: System for the integration of measured and simulated data into production value chain

Outcome:

- Establish a digital material definition for materials data sheets that integrates information from simulation and measurement technology. Such a system will enable procurement specifications for raw materials and methods to qualify these materials before processing. Improved value chain interactions should be demonstrated between suppliers and manufacturers via digitisation of data gathering and the associated procedures leading to higher accuracy and precision of datasets.

Impact:

- Improved information capture about the material supports life cycle management and a circular economy
- Faster and improved product introduction to the market due to optimisation in supply chain processes.
- Increase production rate/volume of advanced and nanomaterials
- Alignment of simulation and characterisation methodologies avoiding now redundant experiments.

5.6.2 Topic 6b: Integration of materials modelling into production and quality control

Outcome:

- A system that underpins the factory of the future by materials modelling in order to supports fast and real-time decision-making.

Impact:

- Increased asset utilisation
- Increased return on capital (ROC) invested in manufacturing equipment and facilities.
- Increased production output
- Quality by design
- Increase production rate/volume of advanced and nanomaterials
- Digitisation of procedures and methodologies integrated with calculations routines facilitates experimentation, reduces error and enhances efficiency of the operation.
- Integration of several testing procedures combined with materials models directly provides a full quality picture.
- Production change overs can be significantly reduced by integrating materials models with standard quality control testing in particularly when moving as an industry towards custom tailored products making product performance an integrated part of the logistics workflow.

5.6.3 Topic 6c New design modelling for improved reliability and sustainability of microstructured materials

Another materials area of high economic or societal impact and with a ubiquitous risk of malfunction is microstructured materials. Thus it is well known that microstructures (e.g. for metals, ceramics as well as for reinforced plastics), can lose their functionality from fatigue or from degradation caused

by wear, damage, fracture and breakage, corrosion, ageing oxidation, thermal stress, flash temperatures, delamination (coatings), matrix failure or fibre fracture (reinforced plastics), separation matrix-particles (metal matrix composites), to name a few examples. The consequences can be fatal. Other challenges of microstructures arise from the fact that the microstructured material's properties depend on the manufacturing process they may have during their transformation to the components (forming, shaping, thermal treatment, welding and soldering, gluing, machining…). Altogether, it is largely unknown how the effect of working environment (such as oil, petrol, biofuels, lubricants, gases, humidity, water) should be considered in the prediction of their performance during use.
Here materials modelling can change the landscape, and there is a need to create models for multiple and combined damage and surface / sub-surface failure mechanisms considering materials properties, specific compound design geometries simulating their working conditions such as load, speed, fatigue stress or corrosion environment to predict their lifetime.

Outcome:

> There is a strong demand for Reliability and Sustainability of Functional and Structural Materials and Components by design. The key is to develop a computational material design tool based on microstructure, leading to the right, desired and required materials properties. The model should take into account the integration of manufacturing steps into the full CMD of components. The main barrier of actual Computational Material Design tools (CMD) needs to be largely expanded and improved in the area of damage, degradation, and failure lifetime prediction, following the approach PSPP (processing–structure–properties–performance). Laboratory accelerated tests should be combined with observation techniques and local knowledge on material behaviour in situ, under operating loads. Models should be robust and built on a strong experimental database.

Impact:

> This approach will have a huge impact in the valorization of EU Products in comparison with low cost countries. Through good product design, European products enjoy high durability in comparison with low cost countries, but there still needs to be an increase in the durability of products to achieve customer guarantee requirements. Design of the materials depends on the conditions of use and durability requirements. If we know how to design the materials in the components for a defined lifecycle and application, then we could be confident, as suppliers and consumers, about the guarantee of a product's life and reliability. Applications needs always to limit the quantity of the materials used (Raw materials directive) and the weight of the components (reduce fuel consumption in transport), and increase performance, higher pressure and speeds (to reduce CO_2 emissions in transport), to increase safety (environmental compatibility and safe use). To achieve all these challenges, we need to design tailored materials for their safe use during a predicted lifetime. In general terms, we advocate ongoing and future research in materials informatics: combining experimental and theoretical high-throughput methods with data mining / machine learning

5.7 Coordination and Support

There is a need for a coordination network in materials modelling that can support

- Integration of material modelling in business decision support systems (BDSS) in industry

- Development of the role of translators
- Establishing roadmaps for model development
- Coordination of existing activities on interoperability of software and operational (open) simulation platform developments in Europe
- Design of a system of databases, validation and interpretation tools Design of case studies demonstrating the potential of materials modelling to industry
- Stimulation of academic software exploitation
- Engagement of SWO
- Development of modelling market place (MMP)

Action(s):

5.7.1 Topic 7a: A network to capitalise on the strong position of materials modelling in Europe and accelerate the transfer of academic knowledge to industrial applications

Outcome:

- The Coordination and Support Action has the goal to network all existing activities happening in the field of materials modelling. The aim is to establish current and forward-looking complementary activities necessary to bring the field of material modelling closer to the demands of manufacturers (both small and large enterprises) in Europe. Materials modelling should become an integral and integrated part of industrial R&D.

Impact:

- Improved accessibility of materials modelling and related databases by manufacturing end-users,
- Increased integration of discrete (electronic, atomistic, mesoscopic) and continuum materials models and databases for industrial use,
- Increased efficiency and industrial effectiveness of materials models in industry and research,
- Establishment of technical and business related quality attributes (Key Performance Indicators) that inspire trust in materials modelling,
- Industrial best practice (methodologies) for end-users increasing speed of development in industries.
- Exposing academics to the importance of integration of basic research into applied engineering for closer and more collaborations.
- Connecting resources, interest groups, model developers and users for greater awareness.
- Significant increase of tailored model development and integration into

Document History

- The first draft of the roadmap was released by the EMMC on 27.09.2016.

References

- http://emmc.info

- “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
- 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.
- „What makes a material function? Let me compute the ways...“, Edt. Lula Rosso and Anne F de Baas. http://ec.europa.eu/research/industrial_technologies/pdf/modelling-brochure_en.pdf%20