The EMMC Roadmap 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 Road Map.

Summary

The Road Map 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). The stakeholders cover the whole spectrum of the Material Modelling Community in Europe:

- *Industrial end-users (manufacturers)*
- *Software owners*
- *Translators*
- *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 2016-2017 should be used to exploit the materials models that exist and focus on successful transfer to the industry to capitalise on the enormous potential and to support this with coordinating networks, integration with business processes, a modelling market place and validation facilities. Model applications are recommended for all LEIT activities as a means to reduce costly experiments and this should be accompanied by transfer of the technology to the participating industries. The EU LEIT Work Programme 2015 contained a Call on model development and the EMMC will undertake activities to establish a detailed Road Map to recommend a focused topic for the Work Programme 2018-2019.

Contents

1 Introduction

This Road Map is elaborated by the European Materials Modelling Council (EMMC [1]). The EMMC has the goal to network all existing 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 material modelling closer to the demands of manufacturers (both small and large enterprises) in Europe.

How was the Road Map elaborated and endorsed?

While elaborating the Review of Materials Modelling, a database for the beneficiaries in 75 NMP projects with materials modelling WPs was created. The coordinator, Modelling WP leader and participants and also the industrial partners formed an initial database of 500 names. These people were invited to share their views. 85 experts representing various stakeholders submitted input in advance of the meeting in writing and 75 experts attended the Policy meeting in February 2014 held in Covent Garden, Brussels. The views were written down in a Report "Materials Modelling: Where do we want to go" published on the LEIT website [2].

The EMMC was created and people who volunteered started various working groups (WG) on topics of their interest and the teams elaborated Discussion Notes as a pre-runner of a Road Map (these are available on the EMMC website [1]).

In the summer of 2014, the database was enlarged and cleaned, keeping interested partners only. This resulted in a database of 600 people who were invited to comment on the above mentioned Discussion Notes. Some 108 people accepted the invitation to come to Brussels on the 5th of November 2014 and discussed and largely adopted the present priorities for Europe.

This was written up in a first draft Road Map which was published on the EMMC website [1] for comments and feedback. Stakeholders were invited to comment on the first draft using the EMMC wiki. The comments received via this discussion as well as via emails etc. have been taken on board in this second draft of the Road Map.

Note that the EMMC Road Map will be renewed and updated in the coming two years to generate the next EMMC Road Map by the end of 2017 and that the database is continuously growing (currently 900 experts).)

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.

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 nanoscale in industry by linking them to the already well-established continuum-models applied to the macroscopic (device) scale. To achieve this objective, the EMMC has so far identified a number of core activities that go beyond the traditional quest toward better, more accurate models, but also reaches out to other crucial elements such as open simulation platforms, information infrastructure, business decision support, databases, multiscale coupling science, education and translation activities, validation and a Modelling Market Place.

The vision of the EMMC is that only when considering all these elements together sufficient synergies between all elements can be created to address the most challenging questions in materials modelling today and the future. 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. There are many challenges that lie along the way, some of them are addressed by this road map, and many more will certainly be unravelled in the future. This road map serves as a starting point and is meant to be a strong basis to ignite further long lasting activities within the materials modelling community and beyond in Europe.

3 Where are we 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, 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 **get answers to very specific questions**. There remain a number **of technical challenges to develop predictive models that are easy in use and affordable yet 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. 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**.

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.

Much development in modelling and its application in industry are hindered by lack of communication and interaction between different modelling communities that may have similar problems. This leads to severe waste of resources and limited use of modellers by manufacturers. The communication needs to be increased and another avenue to connect the stakeholders is 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 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.

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.

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 is rather huge. The explosion of 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 which models, and which software tools are available 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 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 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.

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 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.

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 board.

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 road map 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 Road Maps 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 four key topics (and their subtopics) that need attention at this moment:

5.1 Coordinating Network

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 road maps 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)

Actions: The EMMC advice the EC to open a call for a CSA for a Modelling Coordinating Network

5.2 Integration of Materials Modelling in Business Processes

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.

In the Kick-off meeting of the EMMC the manufacturer stakeholders expressed the requirements and potential benefits as follows:

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.

5.3 Modelling 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.

5.4 Validation of Materials Models

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.

6 Integration of Materials Modelling into Business Decision Support Systems

6.1 Where do we want to get?

In order to better integrate materials modelling into industrial processes and bring modelling on the critical path of commercial product development, a Business Decision Support System (BDSS) is needed. In a global context, making well-thought out decisions on which business strategy to follow and how to best serve ever more demanding customers and fast evolving markets is a very complex process. It typically requires making choices between multiple options both on the commercial as well as the technical side of the business. A business therefore requires, at every operational level, answers to specific questions for making technical and commercial decisions that minimize risk and maximize the success rate of actions. **It implies that tools need to be made available that provide the right data and information based on available data sources and the best possible, state of the art science and technology knowledge accessible today**.

At every hierarchical or functional level, **decision makers more and more make use of materials models** either as App's or as Emulators because they want to understand the issues themselves. Furthermore, decisions made on multiple hierarchical or functional levels require different levels of coarse or fine graining and a tailoring to specific functions and operational needs. **BDSS aims at supporting the development of generic materials multi-objective optimisation tools that can assist commercial organizations do a better job at any level.**

BDSS will be a system that will allow the end-user to integrate materials models with fine-tuned empirical information to address various industrial problems in a pragmatic and reliable fashion. The end-user will be able to for example combine market trends, pricing, customer needs and demands as additional criteria for selecting a specific technical solution tailored to an identified process or product need. BDSS will allow a flexible integration of various materials model types adapted to industry selected challenges that in combination with business criteria define the technically possible and commercially most attractive solution.

The BDSS intention is **not** to prescribe or replace internal established commercial processes specific and confidential for each company, but to create generic tools, approaches, or novel model systems that can underpin with a data driven technical foundation a company's internal decision processes. The eventual use and adaptation of the envisioned tool/methodology development will need to be decided by the end users just like any software available for use today, whether freely available, purchased or licensed. Once the key enabling components for a BDSS are in place, companies will therefore be able to adapt the generic tools to their specific needs without sharing for example their confidential commercial data on customers and pricing or business strategy.

The BDSS objective is born out of the realization that there are many industrial cases where existing materials models are incapable of providing meaningful technical answers to often simple business questions. It implies that decision makers have no or very few tools to assist their decision process (irrespective if they use the model themselves or rely on someone else). The challenge is often related to the fact that there are multiple scenarios possible as multiple objectives need to be satisfied i.e. many technical as well as many commercial ones. For example one litre of milk can be packaged in glass bottles, plastics bottles, plastic pouches, aluminium cans, clay containers etc., each with its specific materials performance benefits and costs (not only financial but also environmental) The question at hand then becomes: How should a company make the best choice for its growth efforts if it decides to operate in this packaging market segment?

The answer requires more than a tabulated materials property and costing comparison, it requires a **multi-objective optimisation** approach where both materials models and experimental data will need to be combined to develop options scenarios and consequences analysis. There are some scientific and technical challenges that need to be overcome in order to create the generic tools and approaches that companies can adapt and use to support their internal, confidential decision processes. The first is that materials modelling applications are not generally ready to deal with the requirements of a BDSS, for example in terms of accuracy, robustness, uncertainty quantification and speed to allow a large design space to be explored.

Another challenge is the massive and ever growing amounts of data and information that cannot be overseen anymore. "The signal is being lost in the enormous noise". Companies want and will need to have the tools to use theirs and others massive amounts of data and all forms of information in a refined, manageable, dynamic and smarter way. Therefore, information and communication technologies (ICT) tools need to be made available to process "big-science & technology and business data" into smart options for data driven decision making that can strengthen the agility of companies, particularly SME's that deal with the massive data/information flows, refine the flow to meaningful and manageable information, and .

The BDSS will involve computational technologies that allow such empirical data to be integrated with virtual materials modelling data. For such an activity novel approaches to materials modelling reflected in new algorithms will be needed. Machine learning, artificial intelligence, and adaptive algorithms are just a few of the possible approaches complementing the existing “chemistry-physics” based approaches.

The refinement of data, the integration of empirical data with materials modelling outcomes, and the reliability of the findings combined with possible scenarios and their business impact are critically important for a successful business operation. In particular for SMEs it becomes a priority that the BDSS also aids in quantifying the overall "risk" of applying materials modelling by addressing issues such as

1. What is the outcome of the materials model?
2. What is the cost associated with applying materials modelling (tools and simulation)?
3. What is the risk accuracy associated with it?

It should however be noted that the tools envisioned are neither aiming at doing a cost benefit analysis of existing or new materials models nor simply connect existing or new materials model. However, there is a need for a generic BDSS system **that targets the appropriate modelling tools around the end-users,** who may not be necessarily modelling experts. In other words this is about "**democratisation**" of the integrated modelling tools - the importance is putting the end-user at the centre so that it's easy to use and develop for the (generalist) end-user. The design of the BDSS thus also needs to address the questions: *who will use the model? A scientist, a researcher, a decision maker? How can inputs and requirements across business functions be included (e.g. supply chain and marketing)?* One key need may be to integrate the market opportunity into a product development process. It should be therefore clear that novel modelling approaches and data processing techniques need combination with “classic” modelling efforts to deliver a successful BDSS!

The large company perspective:

The BDSS should allow an end-user to drive its business to the next level efficiency and develop a business case as fitting into the value chain. The tool should thus allow the collection of information from across the value chain. The BDSS should allow end-users to evaluate the risk of a change of the industrial context of the problem they are working on. Once error estimators for the multiscale modelling states are available, these error estimators could be turned into risk estimators for the performance indicators and are therefore based on materials modelling. The incorporation of business oriented quality and risk attributes call for open interfaces of a BDSS for the integration of purely business oriented context attributes by industry. Optimisation solvers using all quality attributes are an integral part of BDSS software platforms.

The tool should not only present the results of materials models, but put each simulated case in the perspective of the business situation. There is a need for predictive capabilities to convey summary or refined information or options to top management for decision making purposes.

In summary, a BDSS is a novel way to address real and vital needs for decision making on materials use for designing products in an ever more complex future. This challenge is beyond one single company's capabilities and support is thus requested to develop these generic tools, approaches or systems for bringing them from TRL3 to TRL7 where-after all type of companies including software owners can customize them for use in commercial operations. BDSS needs an EU wide approach in particular to advantage EU based SME's.

6.2 How do we get there?

The future of the European industry depends on a strong European-based materials modelling capacity. Such leadership can be expressed and fostered by a funding policy that supports materials modelling-enabled business growth.

Today, it is feasible to apply ICT tools to process "big -science & technology and business- data" into smart options for data driven decision making that can strengthen the agility of companies, particularly SME's. Two important challenges need to be addressed to bring materials modelling to a next level of industrial use.

1. Easy and flexible integration of existing materials models in combination with empirical information to address various industrial problems is a first challenge. Many technical challenges have a complicated multi-variable nature. It typically requires the use of multiple models, each of which may have limited applicability or accuracy. Even then, additional empirical information is often necessary to achieve realistic solutions to the challenge.
2. Secondly, materials modelling applications are not generally ready to deal with the requirements of a BDSS, for example in terms of accuracy, robustness, uncertainty quantification and speed to allow a large design space to be explored.
3. Finally, the combination of simulated potential technical options with the commercial decision making process is a challenge. Market trends, pricing, customer needs and demands are some of the additional criteria for selecting a specific technical solution tailored to an identified process or product need.

Hence there is an industrial need for the development and implementation of methodologies for flexible integration of various materials model types adapted to industry selected challenges that in combination with business criteria, define the technically possible and commercially most attractive solution. These needs can be greatly assisted by the EMMC Material Modelling Marketplace (MMP) and Open Simulation Platform (OSP) activities.

The ideal approach for using such integrated tools in a BDSS would follow the philosophy: *start from the outcome (perhaps a certain consumer-desirable property) and then back-engineer the physical, processing, and additional requirements that lead up to that end-goal.* There will be a **need to define standards and a high level language/set of parameters** that will constitute the backbone of the integration step.

All BDSS components are to be integrated into a single but modular workflow, so that all components are independent, but connectable to each other. This philosophy allows for flexibility of application of the generic tools to different industrial sectors (where the individual components of the workflow may be different). When an end-user is to apply the tool, it should allow for customisation and mirror the operational framework of a company - including all stages of product development. The tool, thus set up with information of all relevant stages, should enable a multi-criteria (objective) optimisation - driving decisions balancing all business needs (e.g. optimised performance and cost-efficiency). Multi-criteria optimisation provides options and may assist in understanding the consequences of a decision for a specific scenario.

The desirable output is a **predictive tool**. Something that can be used to ask the "what if' question, and that can run hypothetical scenarios, which include both the technical and the market inputs for a holistic decision making process. As the link is made with the technical analysis, the output will be the analogue of a SAT NAV for the making a decision, being a choice out of multiple options according to desired selection criteria. These options are the result of optimisation algorithms i.e. best possible compromises between usually conflicting quality attributes. As these optimisation solutions are usually not unique, "what-if scenarios" could be discussed for instance between sales and R&D since optimal technical properties might violate business roles and vice versa as supported by visual exploration tools of the optimal compromises.

One necessary step is to **validate the novel BDSS and component models against measurements, existing data and real financial arguments** (see also the Validation sections). Only this way the BDSS can be trusted. The need is there for a full validation exercise, based on data provided and shared by companies and academics alike.

Translators may advise their customers to use the BDSS and assist in setting up custom made Business Decision Support Systems at particular end-users and may implement the required software components necessary within a BDSS. This is one way to fulfil the Translators role. The setup of technical aspects of an industrial problem, which has successfully been mapped to a multiscale modelling workflow, within a BDSS is a model of the KPI's as functional of the multiscale modelling state variables. The translator may help the end-user in deciding business oriented quality attributes which may depend on the multiscale 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. Translators can thus advice during the BDSS development by communicating specifications learnt in their experiences with end-user decisions.

It is important for Translators while setting up a BDSS to asses and reflect on the decision making process within the industry. This is not unique. In large companies, with “division of labour”, decisions making usually involves several internal hierarchies and each hierarchical level has specific needs for support in decision making. In SMEs the decision making process by contrast may be more direct and the responsibility of single individuals or small groups of people. In any industrial context, irrespective of size of company, risk analysis of a decision is a common and necessary practice. Moreover, the BDSS via the translator can help the end-user in deciding on the resource allocation investments and support in the training and education of the tailored BDSS.

6.3 Actions

Short term actions

- Develop case studies, where integration of different modelling levels (e.g. data modelling, physical modelling, and supply chain inputs) have led to successful decisions.
- Industry players already have modelling success stories which are only present in the "company inside" literature. Ways should be sought to communicate these to the right level stakeholders and decision makers. Such a communication can be achieved using the Material Modelling Marketplace (EMMC-MMP) platform.
- Case studies are to be released and shared, as success stories. This will be a useful exercise to promote this activity and best practice across different business sectors.
- In view of supporting the EMMC initiative a clear statement from companies on successful modelling efforts would provide good PR for management, especially when it is articulated into business relevant case studies. Modelling is not to be confined into a separate section or category but must be an integral part of the decision making process.

Translators can provide:

- Best Practices with clear KPI and ROI
- Initial design of a BDSS: workflows, best practices, Pareto-optimizers (identification of best possible compromises) and tool support for answering “what if” questions.

Modelling Market Place can provide:

- Place to store and archive case studies
- A system to extract multivariable correlations for business decision systems
- Store and facilitate the communication of educational resources for training
- Access to databases of knowledge and expertise to support the BDSS and translation process
- Facilitate the forming of collaborations between different stakeholders
- Facilitate the implementation of new workflows

Medium and long term actions

EMMC recognises that no single company is currently considering financing such a big commitment. Therefore there is the need for sponsoring this activity - either at Member State or at the EU level. The EC can fund the development of the generic tool from TRL3-TRL7 leaving the customisation of the tool to commercial players and other end users. Education in this holistic view is key and the EMMC encourages the EC to promote education towards this goal.

A RIA is recommended for the initial design of a generic BDSS: workflows, best practices in the medium term, followed by the development of a software platform for BDSS, interfaces to model software integration and convenient set up of KPI models; multi-valued optimisation problem solver integration.

7 Translation

Industry will need access to players who have the ability to translate industrial problems into cases to be simulated. These stakeholders should be able to bridge the innovation valley of death starting from the side of the industrial innovation hill by utilizing materials modelling and simulation. This includes the closure of the "language gap" between industrial stakeholders and scientific modellers, and training of the industrial operators during implementation of modelling and simulation at industrial R&D sites. The focus of the Translators is the industrial return on invest and the time to solution. **The credibility of Translators is based on neutral support to implement the appropriated methodology independently from software or suppliers.**

7.1 Where do we want to get?

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 process element in industrial R&D practice based on multiscale materials modelling. Translators are new actors on the scene in an evolutionary sense. As a first step, their role and functioning will be defined and developed fully.

A first definition of their role would be that Translators **start from an industrial problem** and identify a workflow for its solution by using materials modelling. The primary stakeholder within industry interested in a modelling is usually the R&D unit, but the industrial problem is usually set by the high level management or the sales unit. In order to detail the definition of the Translators role in problem solving, it is therefore necessary to understand the industrial context of the problem to be solved, as the context defines the necessary quality attributes of a solution to a problem. These quality attributes will always include time to solution and money to be invested in order to get the solution. Savings in these two attributes are usually mandatory for the usage of modelling at all. The role of Translators includes the identification of all quality attributes, or at least the most important ones, within the language of the context of the technical industrial problem. This implies that non-technical cost measures, like the influence of the solution on the pricing of a final product, and time to market, are taken into account from the very beginning. Within the **translation process**, the language gap between industrial R&D people and modellers, which even exists within industry with a division of labour, will necessarily be reduced.

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 KPI's 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 do their best to identify the best possible tools to be integrated into a modelling workflow. Modelling Software tools, as to be used within the simulation workflow, may include data driven models beside materials modelling software based on predictive scientific models. Translators are aware of the fact that not every aspect of a technical industrial problem may be casted into predictive models, most often for complexity reasons. Translators develop and implement methodologies for using materials models workflows on top of simulation software and available characterisations of materials properties or data, thereby identifying gaps in the available modelling software landscape and data bases.

The Translator's role covers the back-translation of the results obtained by modelling and simulation workflows into the quality and cost attributes defined within the industrial context. 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 both may be estimated using rough estimates, the level of detail necessary in modelling and simulation, and especially the KPI models, during the development phase, need to be refined in order to be useful in technical decision making for R&D people. At all levels of detail, Translators will 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.

7.2 How do we get there?

Within the implementation phase of these KPI driven workflows at industrial sites, usually within the R&D units, a training guide for industrial operators using these methodologies will be developed. Translators are aware of the fact that industrial problems to be solved by modelling and simulation are usually subject to change (and sometimes very rapidly). This applies to the technical problem as well as to the industrial context. Translators support this by using the methodology of change management of requirements.

Best practice guides, evidence on trustworthy, successful case studies and examples of multiscale modelling methodologies for tailored industrial problem solving are the information provided and elaborated by Translators (on the EMMC platform) to convince, with clear neutrality, manufacturers to adopt the multiscale approach. The level of trust in the service provided by Translators will be put on a professional level, similar to services provided by independent consultants in financial industry for example. A code of conduct for Translators will be developed so that manufactures know what to expect from Translators. This code of conduct will be disseminated as the basic definition of the role of Translators.

Last, but not least, the Translators stakeholders within the EMMC will develop methodologies for Translators and translation processes adapted to various industrial sectors. Starting from an initially developed Guide for Translators, which is based on best practices collected within the EMMC, the goal is to develop training courses for new Translators with a focus on how to use materials modelling and simulation in order to support industrial innovation. Attendees of these training courses will get equipped with methods and supporting tools for and thereby effectively enhance the usage of materials modelling in innovations in the European industry.

Specific steps identified so far, necessary in order to develop the role of Translators and to establish this role in industrial innovation cycles are:

- Develop a code of conduct: trust is important. Since Translators need to gain insight into the context of the problem to be solved, a template non-disclosure agreement (NDA) might be useful.
- Document industrial success stories of translation efforts done for instance during project acquisition (big companies and SMEs)
- Retrospectively use these projects in order to identify best/worst practice communalities, set up a best practice guide for translation.
- Develop draft of a methodology for the analysis of industrial problems.
- Translation experiments: use Translators methodology in order to identify necessary improvements on the Translators methodology

7.3 Actions

In the short term, a CSA is recommended to develop the role and functioning of Translators. In the long term, an ITN is recommended for a "Training Program for new Translators" in order to facilitate this important new role within Europe.

8 Modelling Market Place

There is a need for a Materials Modelling Hub, a place for information exchange on key issues concerning materials modelling and its industrial application. There is a lack of a platform that is focused on exploring possibilities of, and offering 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 exchange between the areas of fundamental material modelling and their potential end-users are at present one of the major obstacles for further progress of material science. **There is therefore an overarching need for a platform that manages the materials modelling infrastructure.** A Modelling Market Place containing databases and libraries of models and data, validation and educational resources will fill this need. Such a platform will assist and further strengthen R&D foundations in Europe ensuring its continued leadership in advanced technology and modelling.

8.1 Where do we want to get to?

As outlined above, there is a need for increased communication and another avenue to connect the stakeholders is required. In future we envisage 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). This would be completed with an explicitly named contact individual from the software owner who is responsible for producing and maintaining the model.

The Modelling Market Place (MMP) will be 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.

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 material modelling in industrial problems. The MMP would contain 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 1 for the proposed structure and contents of the MMP.

The various databases will 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.). MMP is therefore **a gateway to material modelling and its "big-data".** Systematic data mining (e.g. by artificial intelligence, model reduction, quantitative structure/activity/-property relationships, etc.) could represent a promising approach for fully exploiting the potential of collected (Big-) data.

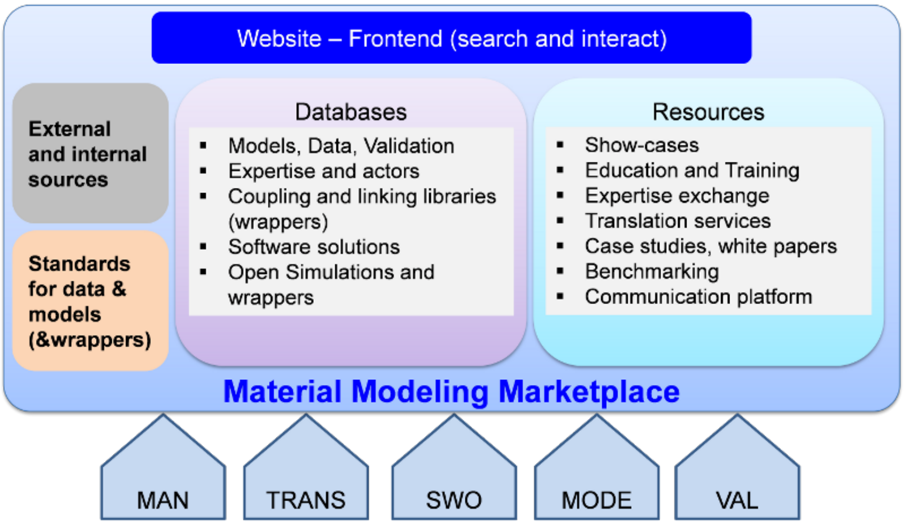

Figure 1: A schematic structure of the various components in the Material Market Place and relation to stakeholders.

The requirements to protect intellectual property will need to be 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 MMP. The degree of openness of the data in the MMP 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.

The MMP should enable coupling/linking of all components in and effective, easy and maintainable way. Standards are needed for optimal information retrieval and interoperability of different components. Standards are 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. 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 standards. The MMP will also enable data quality to be tested 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 MMP will make it possible to publish data, models and early results. Each such publication on MMP will have a unique identifier that can be cited.

Benefits to stakeholders

The wide availability of a Market Place providing access to all information on material modelling and as well as possibilities for collaboration and communications will accelerate and advance material modelling design and deployment in the EU. 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.

Benefits to Manufacturers (MAN) include

- Mapping of available modelling activities and resources in EU
- 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.

Benefits to Translators (TRANS)

For TRANS, the MMP will offer 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 MMP is that it offers:

- A communication channel
- Databases of models, software tools and materials data and uncertainty.
- Databases for case studies, white papers and webinars

Benefits to Modellers (MOD)

MMP will also provide value to MOD in a number of ways, including:

- Enhance dissemination in the academic simulation community

- End users can publish and access modelling results using the databases and show cases
- Each publication on MMP will have a UUID/URI (unified universal ID, universal resource identifier)
- 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

8.2 How do we get there?

The MMP will require input and involvement from all stakeholders. MMP 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. An operational simulation platform will assist by promoting the use of software wrappers that are needed for databases so they can talk to each other. The involvement of the SWO in this is desired. Translators would assist in identifying the intended audience of MMP; this makes a huge difference in the appearance of for instance a web page. Translators should also get involved in actions of the MMP.

8.3 Actions

Short term actions

Continue current EMMC-MMP actions:

- 2Q.2014: creation of a media-wiki collaborative site for the EMMC, Registration of domain name wiki-emmc.org
- 3Q.2014: Registration of the emmc.info domain name
- 3Q.2014: Kick-starting emmc.info (modest but functional website)
- 4Q.2014: Web-based registration form (php+html5) to collect initial member data found

Additional short term actions:

- 1Q.2015: Initial survey of available database and content management systems and suitability to the MMP requirements
- 1Q.2015: initial requirements and USE CASES for the future MMP site (including databases of models, data and wrappers)
- 1Q.2015: Move the wiki-emmc.org and emmc.info into one home
- 2Q.2015: Publishing new form/questionnaire for the database of actors (DBA), to be linked with the wiki and emmc.info
- 3Q.2015: Publishing the first component of the MMP: DBA
- 2015 and beyond: assembling and coordinating existing activities related to the wrapper and databases requirements and operations within EMMC
- 1Q.2015 MMP will start investigating the IT behind existing databases and start designing a common interface (experiment on wiki-emmc.org and emmc.info)
- 3Q.2015: Meta-database of models (input, software descriptions, stakeholders)
- 4Q.2015: linking the model database to the DBA: first version of the marketplace

Medium and long term actions

- A CSA is needed for assembling and coordinating activities starting from 2016/2017.
- RIA projects or one big IA are needed to implement a set of standardised, clustered databases.
- In the CSA action:
    - Concentrate on assembling and coordinating existing activities related to the resources and databased of wrapper operations for simulations and databases.
- Support from EU projects with materials modelling Work Packages to provide data for the various parts of the MMP and to contribute to discussion and the structure of the databases, data standards and data managing (archiving, linking, publishing, retrieving, metadata schemes, analytics, etc.)
- Encourage projects to allocate resources for specialized computer scientists and software engineers
- It is recommended that the EU stimulates to include elements of data mining and statistics (based on databases) in combination with scientific and engineering tasks
- It is recommended that the EU encourages EU projects to collaborate with the EU-MMP and that they recommend that new projects results should be uploaded or linked within the MMP site
- A model selector of the MMP is to be designed and agreed with all stakeholders

9 Design of a System of Databases

9.1 Where do we want to get?

The overarching goal of the EMMC in this domain is to establish leadership in "sharing data across modelling fields". Subfields of modelling as well as experimental science will develop increasingly mature databases for their own fields. In these databases, both simulated and experimental data are gathered. 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. Nevertheless, internal structures and data formats are driven by the individual community and the belief is that the subfield databases should remain structured as the subfield has designed them to satisfy their purpose. 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. Scientific results are published 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.

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, 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.

9.2 How do we get there?

Metadata should be elaborated to describe and share the information in the different subfields so that a catalogue can be built of available data in the repositories scattered across Europe. These metadata could also be the basis of an exchange methodology between databases and models. This should alleviate the current incompatibility or incompleteness of the set of distributed databases.

- Databases

  The proposed approach is in incremental small realistic steps, taken one at a time. Databases are a sensitive issue and there is a need to grow trust which in its turn will reach wide participation. Two similar approaches are proposed for simulation data and for experimental data.

  - Requirements and design of a <u>database with simulation data.</u>

    This activity addresses the technical task of cataloguing what exists with agreed metadata, without the wish to restructure any subfield! The content addressed can be elaborated in three steps:

    Step 1: Database of simulations (metadata on code and input)

    Step 2: Databases of simulations (input, code, and raw output data)

    Step 3: Database of materials properties (processed model output)

    Timeline: Proposal for metadata in 2016, start of coordination activities in 2017

  - Requirements and design of a <u>database with characterisation data</u> (raw data)

    Step 1: Database of measurements (metadata on equipment and measurements)

    Step 2: Databases of simulations (equipment and measurements and raw output data)

    Step 3: Database of materials properties (processed measurement output)

  - Interface modellers-experimentalists

    Modellers should define guidance for data needed for validation of their models

Later on it should be discussed whether actual databases should be assembled in a central place. First the end user specifications for such a database should be established. Then the scientific requirements and software requirements for each workflow in multi-model simulations, open simulation platform should be addressed. These activities should work in close cooperation with standardisation activities.

Reproducibility of simulation data is not always guaranteed, especially if the applications or hardware used to generate it originally changed. It was suggested that virtual machines would be created to archive not only the data and related models, but also the software (and the original operating environment) that was used to generate it. This may require special licenses from proprietary SWO to allow storing, when needed, also the specific version of their software for the purposes of archiving and reproducibility.

- Requirements and Design of Website facilitating beta testing of codes under development

  Timeline: earliest 2018-2019
- 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

9.3 Actions

The development of the databases is proposed to be part of the CSA on networking for the initial design and to be part of RIAs or an IA for the new market modelling place.

The CSA should take on the role to actively stimulate participation in the database activities.

10 Model Development

10.1 Where do we want to get?

Better, more accurate, reliable and efficient models and methods

Developing more realistic, i.e. more reliable, physics/chemistry based models to generate the data is of great importance. The lack of predictive modelling, along with the lack of efficient methods and easy-to-use applications is one of the biggest gaps of all hindering more industrial use of modelling. For example, a survey of existing models and their capabilities (taxonomy) for mesoscopic models is being conducted. This activity highlights the need for databases as a mechanism to identify gaps. There is a wide agreement that an analysis of necessary material model development for specific problems relevant to industry needs to be conducted.

In industry we need to link models describing phenomena at small scale (e/a/m models) to the device/application (continuum models). Widening separate models and linking and coupling should go hand in hand. Reliable coupling and linking recipes for materials modelling are often as sophisticated as the individual models themselves. Infrastructure to enable the linking and coupling, especially open simulation platforms (OSP) and integration is much needed as it will enable such coupling and linking (C&L). Existing knowledge (models, data, characterisation and validation) is part of the process of materials modelling, hence in addition to the need from an open simulation platform a need exists for an integrated system with databases.

A tight connection between the materials models and experimental characterisation needs to be established to allow modellers to update/enhance their models and to communicate the quality boundaries of the model to the end-users. Influence of the quality of one model on results of subsequent models if used in a multi-model chain should be documented and communicated for industry relevant scenarios.

A workflow hierarchy is proposed that should be promote to bring modelling closer to business decision support systems and use in industry

1. Models and model development: leads to database of models and simulation data.
2. Coupling and Linking of models: leads to new multiscale science, enable to model phenomena that cannot be described by one scale alone.
3. Validation: to deliver information on the applicability and accuracy of modelling (and in some cases augment modelling data with experimental sources).
4. Integration of models (using the OSP) and databases infrastructure (MMP/DB): enable the modelling of device and process level systems

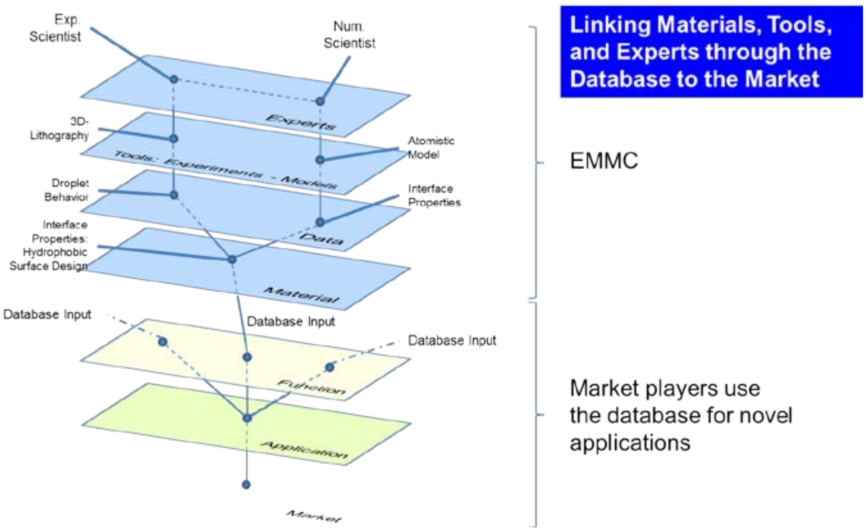

Figure 2: A schematic representation of the interplay between modelling, validation, and databases as well as expertise.

Cross correlation between different workflows and data can lead to standardised/harmonised approaches. Such a cross correlation, where both modelling data and sources are coupled is shown in Figure 2.

While the processing of materials is not shown in the illustration in Figure 2, it is acknowledged that processing has a strong effect on the material properties. In addition, any property of material should be documented by a set of data over wide in service conditions. This set of data should be provided with a sensitivity analysis, depending on the variability in the processing (e.g. process temperature range varies by 2%). This would contribute to trust in the values documenting materials.

10.2 How do we get there?

The EMMC is to undertake road mapping exercises to identify the gaps to be filled in widening models and methods and prioritise them. It was suggested to reiterate a pure model improvement Call in WP 2018-2019, which is to be prepared by a Road Map on the issue. This could be justified by the huge number of proposals submitted for the 2014 Call (making the success rate very small). Therefore calls or actions targeted at “widening models” (where model is as defined in the modelling review brochure [4]). It is recognised that “extending simulation methods" to give more accurate and efficient solution strategies of existing models is part of the DG CNECT programmes. It is also recognized that error measures need to be treated (in conjunction with widening models and methods as well as with validation).

10.3 Actions

A CSA is recommended to set up a Road Map with an analysis of necessary material model development for specific problems relevant to industry need to be conducted. Existing mesoscopic modelling approaches should be categorised according to the most relevant features, namely the granular description, and those models without should be excluded. The Road Map should also include novel coupling and linking methods. The analysis should be conducted across the board.

11 Coordination of European developments on Interoperability of Software and Operational Simulation Platform

11.1 Where do we want to get?

Industrial problems can only be solved using several materials models together and there is a need to orchestrate the interplay of different software tools. Not only the interoperability of software but also their linking to experimental databases needs to be investigated. Many academic and commercial modelling software packages exist and a number of manufacturers have expressed the wish for an open simulation data exchange format allowing the integration of software from different sources. Specifically, there is a need for a bridge between the process scale of the component and electronic/atomistic/mesoscopic models. The combination of tools requires a standardised information exchange in order to be efficient. There is a need to coordinate the activities in this field conducted in EU projects and other activities so that communication standards can be agreed by all stakeholders.

There is a need to globally coordinate the specification of standards to avoid fragmentation. Active participation of software owners and manufacturers in setting the needs and requirements for acceptable standards is important. Software owners and Translators should participate in the standardisation and open platform actions in order to express the needs of the industry that require that all the models and databases they need are smoothly operating together. Some international activities within the Integrated Computational Materials Engineering (ICME) community to coordinate a global standard (JP, US, EU, KR, and IN) are on-going and this needs to be enlarged to other fields.

An EU wide action for communication standards is essential, otherwise EU software owners and manufacturers may be faced with de facto international standards that do not take into account the special needs and interests of EU software owners and manufacturers, posing a threat that may undermine their competitiveness.

An operational and open simulation data exchange format will present an added value to the workflow of material design and is poised to increase the reliability of modelling. This should also support the integration of material modelling into business processes.

To have a low threshold for the adaption by academic and SME software developers, the basic communication (metadata) between the varieties of software tools have to be standardised, made open and must be freely communicated to all stakeholders. This standard could then be supplemented by a standardized file exchange. The communication and file exchange standards should then be used to develop an open simulation platform. The platform in this context essentially is understood as the tool orchestrating the different codes from different vendors, but it does not contain the codes themselves. Open Platforms are thus not meant to replace any existing market solution. The "Open" in "Open Platforms" does not refer to "free" integrated tools, but rather to the openness of the data formats, which is a prerequisite for integration. Software vendors are expected to profit from an open platform concept allowing a modular integration of their specific solutions with software already in use at manufacturing sites. The EMMC believes this will strongly increase the exploitation of all existing software tools - academic and commercial – of all four classes- in

Europe. It is further believed that the combination of these tools in a platform structure will lead to new insights and to the development/qualification of new options for materials and processes at a much higher pace.

The EMMC thus requests the EC to recognize this European-wide interest and to fund interoperability activities including an open simulation platform and support its development from TRL3-7 () after which each software vendor can customize the result and commercialise it).

11.2 How do we get there?

A 10 year planning would involve **(***Timeline: 2015-2025*):

1. developing the metadata standard (e.g., keyword bases) for models
2. creation of technical basis for Common universal/unified Data Structures (CUDS)
3. publication of the CUDS specifications

Together with the Modelling Market Place we should

4. assemble(information on) software tools covering all scales and stimulate the development of wrappers for them
5. assemble (information on) solvers used to solve the physics equations and ensure they can be integrated into the platform
6. assemble (information on) data processors like homogenisation tools including volume averaging etc. and ensure they can be integrated into the platform
7. assemble (information on) “estimator tools" and ensure they can be integrated into the platform
8. assemble (information on) wrappers
9. reflect on database technology

11.3 Actions

A CSA is recommended to agree and promote communication standards (as a start, first at EU level) between EU software owners, manufacturers and modellers.
A RIA is recommended to design a new system that can integrate materials modelling components used in industry.
It is advised to allocate efforts in EU-LEIT projects on the use of standards and actively contribution to their development.

12 Validation of materials models

Industry requires validated material model workflows. Materials modelling should be an integral part of a Business Decision Support System. Thus quality attributes of the solution is determined by technical as well as business aspects (like time to solution and money to be invested). A facility to coordinate the necessary characterisation and validation methodologies is needed. This chapter deals with experimental data and its use to validate materials models. Databases are discussed separately in an earlier chapter.

12.1 Where do we want to get to?

Raw experimental data can be used in validation after the calculation of materials properties. This can be difficult and demands good theories, including homogenisation. The generation of materials properties from the raw data is a field in need of development for industrial use and is an area of materials modelling which is often as challenging as the generation of the raw data itself. Tools need to be developed which extract the information from raw data which is standardised and linked.

Validation should be done against application ranges of industrial relevance. Translators may help to define such ranges. Since many models need experimental results for their initialisation, validation should include sensitivities of the validation results against experimental uncertainties. These sensitivities may be transformed into a reliability analysis of the solution generated by modelling workflows.

Optimally, databases need to be expanded with the more accurate, reliable data as soon as the model/method development enables this.

It is emphasized that the curation of the experimental databases used is very important for the validation. The quality of the data needs to be continuously challenged to prevent stagnation of the use as reference data. For the validation of various models, tags are needed and high quality documentation of the experimental data using agreed metadata.

Raw experimental data is suggested to be stored to allow modellers to do renewed validation exercises on the same data. The use-frequency of the data (number of downloads and possibly related activity, e.g., use by MMP components) will indicate its quality. In this way raw data will be disconnected from the interpretation. The availability of the data will actually allow, with the proper tools, to uncover new aspects to be investigated and conclusions to be drawn. The process how raw data was obtained needs to be specified. There is a need to make a distinction between primary proto raw data and processed data (proto data to which model was fitted).

The process how raw data was obtained needs to be specified. Efforts must be given to store also the workflow, so that data does not lose its relevance, or become 'bricked' i.e., useless, because it will become impossible to track it back.

12.2 How do we get there?

It should be agreed with all stakeholders what metadata is meaningful. Further research into this question is needed.

12.3 Actions

A CSA is recommended to design a validation infrastructure to enable:

1. Data description, data handling, including data mining and linking data
2. Calculation of materials properties from the raw experimental data

3. Development of new test facilities/devices and experimental protocols adapted to the needs of validation.

RIAs or one large IA is recommended to develop the content of a virtual EU platform of laboratories able to carry out experiments and validation of models.

13 Design of Case Studies

13.1 Where do we want to get?

It is recognized that case studies are important to convince industry it is worthwhile to invest in material modelling. Use cases and case studies will also determine what features shall be integrated in the new generation system for material modelling and also how the user interface will look like. Likewise, use cases of the data is key to determining the requirements of the databases (validation, MMP, etc.). Strategic coverage of Industrial demands should be ensured by the set of case studies. Eventually, the community should be able easily to access any publication (peer-reviewed or non-proprietary reports) which presents either success stories of materials modelling or critical situations where modelling failed in predicting the right response (leading to requirements for model improvements).

Keywords to classify the case studies categories should be agreed. These cases should be guided by the requirements of target industrial audience and should include:

1. Use of materials models and databases in an industrial environment
2. KPI models, benchmark problems

13.2 How we get there?

Translators may be able to identify Use Cases of modelling software tools including databases based on their experience with industry.

13.3 Actions

An initial set of case studies will be created by the EMMC based on input from the Manufacturers stakeholder group.

A conference could be organized by EMMC focusing specifically on how to replace test setup and mock-ups by numerical simulation.

A CSA is proposed to collect and elaborate further case studies, including success as well as failure examples

14 Stimulation of academic software exploitation

14.1 Where do we want to get to?

The purpose of the LEIT programme is to transfer academically developed software to industrial use. It has been recognised that there is a need to produce better structured software and this holds in general for the code, data standards and integration of codes. Three phases in software development can be distinguished:

- **PHASE I: Exploratory phase** (new functionality of models)

  In this phase new models are elaborated with new physics/chemistry, and the models are applied to one or two specific test cases. The development is more science oriented. Exploratory model development takes place mostly in academia. Software developed in this stage is typically not user-friendly and is often shared freely among specialists (mostly academics) through PhD and postdoc collaborations. IP protection is usually only covered by the academic code of conduct. The ideas are often the basis for literature articles.

- **PHASE II: New material modelling software**

  In this phase new material modelling software has been validated on a set of test cases and has thus proven wider applicability and the software has the ability to solve new problems of value for industry. The software is in a prototype phase. In the later stages of this phase, the software is used by a wider community and applied to a wider range of systems.

- **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. Companies ensure full validation, documentation, user-friendly interface, testing suites, durability and **long term support systems** are developed since the life span of the successful models is many decades.

The target of EU-LEIT research and innovation funding will be to reach Phase II in their projects since it will 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 precise?
    - Is the solution easy/possible to get in an industrial framework?
- Software quality is a.o. determined by:
    - Stability and resilience
    - Performance (CPU and memory requirements, etc.)

  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:

- 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 distributes

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 academicals 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.

14.2 How do we get there?

Guidelines for good software engineering should be formulated and should be adhered to in projects. Workshops on basic software writing should be recommended for new modellers as well as workshops on version control and testing suites.

There should be a stronger emphasis on the application of best practices, standards etc., in public funded project.

14.3 Actions

- SWO to organize a white paper on software quality and software engineering advice.
- TRL's specifically designed for software development should be developed based on the H2020 TRLs
- The EMMC should make an inventory of the training on software engineering available.
- The EMMC should agree a whitepaper on licencing recommendations agreed with all stakeholders
- The EMMC should elaborate communication actions towards academic developers concerning drawbacks and pitfalls of different licensing schemes.

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.

References

[1] http://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] 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.

[4] „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

[5] HORIZON 2020 - WORK PROGRAMME 2014-2015 general Annexes. http://ec.europa.eu/research/participants/data/ref/h2020/wp/2014_2015/annexes/h2020-wp1415-annex-g-trl_en.pdf