EMMC Roadmap

Materials Modelling and Digitalisation of the Materials Sciences

EMMC ASBL

The European Materials Modelling Council

Responsible for content:

EMMC ASBL

Avenue Louise 54, 1050 Brussels, Belgium
CBE no.: 0731 621 312

The EMMC Roadmap for Materials Modelling and Digitalisation of the Materials Sciences

October 2020

Editors:

Nadja Adamovic, Jesper Friis, Gerhard Goldbeck, Adham Hashibon, Kersti Hermansson, Denka Hristova-Bogaerds, Rudy Koopmans, Erich Wimmer

Content

Executive summary 6
  Providing the toolbox ("Content") 6
  Making modelling readily accessible ("Framework") 7
  Creating Industrial Impact ("Implementation") 8
1 Introduction – Preamble 9
2 Providing the toolbox ("Content") 12
  2.1 Model development and validation 12
    2.1.1 Industrial Need 12
    2.1.2 State of the Art 13
    2.1.3 Gaps 14
    2.1.4 Definition of success 16
    2.1.5 Recommended Action 16
  2.2 Interoperability and integration 17
    2.2.1 Industrial Need 17
    2.2.2 State of the Art 18
    2.2.3 Gaps 20
    2.2.4 Definition of success 20
    2.2.5 Recommended Action 21
3 Making modelling readily accessible ("Framework") 22
  3.1 Data repositories and Marketplaces: Materials Knowledge and Information Management .. 22
    3.1.1 Industrial Need 22
    3.1.2 State of the Art 23
    3.1.3 Gaps 23
    3.1.4 Definition of success 23
    3.1.5 Recommended Action 24
  3.2 Translation and Training for Companies 25
    3.2.1 Industrial Need 25
    3.2.2 State of the Art 25
    3.2.3 Gaps 26
    3.2.4 Definition of success 27
    3.2.5 Recommended Action 27
  3.3 Industrial Software Deployment 28
    3.3.1 Industrial Need 28
    3.3.2 State of the Art 28
    3.3.3 Gaps 29

3.3.4 Definition of success ... 29
3.3.5 Recommended Actions ... 30
4 Creating Industrial Impact (“Implementation”) ... 30
4.1 Tools ... 33
4.1.1 Industrial Need ... 33
4.1.2 State of the Art ... 33
4.1.3 Gaps ... 34
4.1.4 Definition of success ... 34
4.1.5 Recommended action ... 34
4.2 Data generation, qualification and validation ... 34
4.2.1 Industrial Need ... 35
4.2.2 State of the Art ... 35
4.2.3 Gaps ... 35
4.2.4 Definition of success ... 36
4.2.5 Recommended Action ... 37
4.3 Processes ... 37
4.3.1 Industrial Need ... 37
4.3.2 State of the Art ... 37
4.3.3 Gaps ... 38
4.3.4 Definition of success ... 38
4.3.5 Recommended Action ... 39
4.4 Workforce Engineering /Talent Development ... 39
4.4.1 Industrial Need ... 39
4.4.2 State of the Art ... 39
4.4.3 Gaps ... 40
4.4.4 Definition of success ... 40
4.4.5 Recommended Action ... 40
5 About EMMC and this Roadmap ... 41
5.1 Disclaimer to the approach ... 41
5.2 EMMC- European Materials Modelling Council ... 42
5.3 Stakeholders ... 43
5.4 Vision ... 44
6 Acknowledgements ... 45
7 References ... 45

Executive summary

The EMMC Roadmap defines a path forward for materials modelling and digitalisation of materials sciences. It is the culmination of five years of knowledge- and experience-gathering, by the EMMC, on the needs of European materials industry in the modelling field. The EMMC Roadmap acknowledges the significant progress that has been made over the past years, but equally identifies gaps, and provides direction for achieving the ultimate vision of: Having an agile European materials industry with intelligent enterprises that maximise and integrate the utility of digital materials sciences knowledge.

The future success of a European manufacturing industry depends on remaining innovative and competitive in a global economy. Modellers, materials data scientists, software owners and translators need to be aware of their interdependence and become enabled with the necessary tools to achieve the vision for the European manufacturing industry.

In the Roadmap, the key topical areas that can maximise the impact of materials modelling and digitalisation of materials sciences for industry have been critically assessed. For each, the current shortcomings, in relation to identified industry needs, are defined in detail as to the state of the art and the remaining gaps. Recommendations for actions are made to overcome the gaps. Successful follow up actions can thus lead to a positive advancement of materials modelling and contribute to the overall ambition of establishing a strong and agile materials related industry in Europe. Many aspects need considering both on a technological and an organisational level, which requires talented people in multiple disciplines. Making it happen becomes a complex interplay between the required materials modelling toolbox (content), how modelling is made available and readily accessible (framework), and how both can be used to address the defined needs (implementation) of European materials industry.

Providing the toolbox (“Content”)

Efforts to understand the nature and workings of materials through science and technology remain the essential feeding ground for modelling and digitalisation of knowledge. Either theoretical considerations or sets of data organised in a logical sequence can lead to models. Mathematics in combination with the multi-scale aspects of materials and their functionalities can lead to capturing relationships and algorithms that segment modelling into a discrete and continuum space. Content creation is a continuous and ongoing effort that needs future support, having two aspects:

Model development and validation

As materials modelling capabilities, as well as the interest from industry, keep growing there is a need for trustworthy models and workflows that manage to handle industrial problems. This is a challenging task given the complex scenarios of the real world. Significant model development and validation actions are needed while at the same time there is a need to promote a wider exploitation of the best available, already existing, models and workflows. Fortunately, modelling and model development are currently becoming ever more commoditised and powerful through better domain knowledge, novel workflows and algorithms and increased computational power.

Interoperability and integration

The multi-scale and multi-materials aspects of materials products may require that models at different levels of sophistication need integration to ensure interoperability of the underlying algorithms. This remains a critical aspect to ensure successful product and application developments. The key fundamental goal is to find strategies to match and communicate materials properties and phenomena between different levels. Here the development of a common syntax can provide valuable logistic help and needs fostering at different levels of sophistication with the over-arching goal of a workable ontology for materials modelling efforts as a whole.

Making modelling readily accessible ("Framework")

To operationally implement materials models and workflows, an environment needs to be created that ensures model access, use, and application. By default, it requires powerful computational hardware and software that enable meaningful use of models to create new knowledge and data, and the mining of existing data. Furthermore, a framework for results representation, interpretation and storage is needed. Altogether, enabling and promoting materials modelling and digitalisation of materials sciences also include emphasizing the aspects of:

Data repositories and marketplaces

Data are critical to meaningful modelling. Data come in different shapes and forms either experimentally generated or simulated and together with their so-called meta-data need to be validated and stored. Getting access to the right and validated data, over the extremely broad spectrum of materials, is a major challenge that requires a meaningful organisational approach and an appropriate infrastructure. The same applies to the models itself: being available for access and validated. The combined data and model's availability in a marketplace built on FAIR (Findable, Accessible, Interoperable, Re-useable) principles[a] is essential to effectively use the pooled knowledge of relevant science and technology.

Translation and training

The complexity of models in terms of what they bring and how to use them requires that important efforts are needed to translate a perceived problem or challenge into a setting that can be addressed by the right models and data sets. Facilitating the access and use requires training in understanding the need, identification of the available trainers, and the eventual delivery of the results in a meaningful language to the problem owner.

Industrial software deployment

Coding an algorithm for use as a model that possibly enables simulations can be done at several levels of being "user-friendly". However, to be useful in an industrial setting, the operational part needs to be very functional i.e. the user must be able to focus only on the problem solving and not on the operational intricacies of a model. Continued efforts need to be made to advance the models and to reduce the threshold of their use combined with the understanding of what the model can and cannot bring. High-quality long-term support is essential for successful industrial deployment.

---

[a] https://www.go-fair.org/fair-principles/

Industrial integration and economic impact

In industry, similar to the ability for integrating data and models, a strong drive exists for more and better fact-driven decision making. Companies, to ensure their sustainability, require decision making that combines not only materials technology insights but equally environmental and socio-economic aspects. Companies want to maximise their economic impact for which the combination of data analytics and model simulations can be extremely time saving and enable better decision making.

Creating Industrial Impact ("Implementation")

The goal of the Roadmap is to further the industrial impact of modelling. To that end, it provides direction on implementation measures to put content and framework to the test of practical use. This includes several aspects of actions that can be very specific to the different manufacturing industries or market segments. Nevertheless, in industry, the operational context and drive for implementing materials modelling and digitalisation of materials knowledge is driven by production and product requirements and not necessarily by the specifics of context or framework.

Models, methodologies and optimisation approaches

Industry requires engineering solutions for identified challenges that can be tool box based but with equal emphasis on empiricism (data-driven). It becomes necessary to have flexibility in toolbox selection and composition. Furthermore, the industrial emphasis is typically on "what ifs", which require simulation and emulation with focus on the results as options towards solutions.

Data generation, qualification and validation

The competitive nature of industry requires emphasis on proper data security and on ensuring confidentiality and intellectual property rights. It sets additional standards on the data generation, qualification and validation that need considering when implementing a modelling strategy.

Collaboration frameworks and Infrastructure and workflows

The multifunctional nature of industry may set demands for collaborative networks operating with a specific infrastructure and workflows. Material modelling needs adaptation to such environments for a successful implementation and use.

Workforce Engineering/Talent Development

Ensuring the continuity of industry requires talented people. In the specific field of materials modelling and digitalisation of materials knowledge a major emphasis needs to be put in place to attract the necessary and the capable people. Promotion of the skills necessary, with emphasis on future employment, requires visibility of the opportunities, talent development efforts, and education, and familiarisation with the topic, early.

The Roadmap sets the direction and presents pragmatic approaches for assisting industry to successfully implement materials modelling and digitalisation of materials knowledge in the coming years. It includes Recommended Actions relevant to all Stakeholders, in particular for consideration by the EU Commission in the Horizon Europe framework program.

1 Introduction – Preamble

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

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

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

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

Numerical simulation in industry today is mostly dominated by continuum Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) models solved by Finite Element or Finite Volume Analysis. These continuum models form part of the Product Lifecycle Management/Computer Aided Engineering (PLM/CAE) process which started more than 50 years ago and is regarded as a mature discipline. PLM/CAE is widely adopted in industry and is served by a number of multi-billion Euro software companies.

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

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

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

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

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

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

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

Numerous modern numerical methods and software packages have been developed both by academic and industrial parties that allow fast and reliable simulations of many materials properties and systems for a large variety of technological processes. Also, there is wide range of traditionally separate communities engaged in the various modelling activities, including electronic, atomistic, mesoscopic and continuum models (e/a/m/c) in Europe. The explosion of the number of models (of mostly the materials relations, and the data related to these models) makes it difficult to find the most relevant solutions in a timely manner and it is often unclear which models and which software tools are available for a particular physics/chemistry or technical problem. There is currently no widely agreed platform standard that manages the wide range of materials informatics (model and data) infrastructure.

In addition, even when specific models are available, they often do not fulfil the needs of modelling and simulation of interrelated engineered systems in an industrial context involving complex decision-making processes[1]. It is very hard to link and couple them for closed loop optimisations. For example, in manufacturing processes where material properties are defined, components are designed, and quality assurance and evolution of properties must be conducted during service.

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

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

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

2 Providing the toolbox ("Content")

2.1 Model development and validation

2.1.1 Industrial Need

Perhaps one of the most serious barriers to the adoption of modelling in industry is lack of confidence in the modelling results, i.e. lack of confidence in the accuracy of the models and workflows. This is tightly coupled to the difficulty to treat real complex systems in a realistic fashion and in sufficient detail. For electronic calculations, for example, achieving total energies with an accuracy of 1kJ/mol or 10meV, which is needed for certain crucial industrial applications of complex systems, remains a fundamental challenge. Overcoming such barriers should be one the major thrusts of future research.

Furthermore, there is an increasing need for *tailored* bottom-up materials design and there is a growing use of complex nanostructures that provide *tailored* functionality. Modelling using discrete-particle models (*electronic, atomistic* and *mesoscopic*) can in principle provide such capabilities and unique detail, i.e. high-resolution particle-based information about functionality and mechanisms. However, because of a range of barriers, the application of discrete models remains an unrealised vision (and therefore less urgent/interesting) in many industrial sectors, while in others it is already a reality. There is a great need for improved methods and workflows that generate such detailed information for complex systems at a reasonable cost.

As data-driven approaches enter the materials modelling field there is a certain optimism that the combination of physics-based and data-driven approaches will constitute an interesting opportunity for substantial gains in speed and accuracy. There is a need to continue to explore the synergies between the two strategies and the workflows that make use of them.

Materials models, or more precisely the materials relation part of the model (see CWA[b]), are often developed to describe a material in a certain window of applicability and there is no guarantee that applications outside of this window shall deliver accurate, reliable or even qualitatively correct results. There is a need to routinely subject materials models, and in fact the entire workflow to a formal

---

[b] CWA on Materials Modelling - Terminology, classification and metadata: ftp://ftp.cencenelec.eu/CEN/Sectors/TCandWorkshops/Workshops/WS MODA/CWA_17284.pdf

validation and verification (V&V) process. This can save money and time, and help the process of innovation. However, while the V&V process is generally well developed for continuum models, for discrete models as well as for multiscale modelling workflows there is a need for verification and validation guidelines.

The V&V protocol requires credibility assessment procedures which rely on robust measures of uncertainty quantification. There is a need to develop the V&V processes especially for discrete models with the support of advanced uncertainty quantification (UQ) techniques. Improved and more robust UQ is urgently required for discrete models in order to develop the necessary reliability of credibility assessment procedures.

There is a need to increase the capabilities of, and confidence in, Coupling & Linking (C&L) methods by improved modelling protocols, and improved accuracy metrics (V&V, UQ). A standardisation or at least a systematic approach to the assessment of C&L accuracy would be highly beneficial to their adoption. Making such capabilities available to industry would induce an increased trust into C&L methods.

2.1.2 State of the Art

Model(ling) accuracy. While materials modelling techniques have had unprecedented success and been applied to timely applications in a range of industry-crucial areas, it is rather the rule than the exception that real systems are extremely complicated and the models available are not guaranteed to yield results of an adequate accuracy. Industry cannot afford to use models and workflows which give unreliable results, and it is of highest importance to improve the accuracy of models and methods, and to do so in a consistent and sustainable way. Moreover, especially for ab-initio and atomistic models the a-priori estimation of errors is currently lacking. There is a large shortage of funding nationally and at a European level for materials model developments.

Physics-based vs. data-driven. EMMC surveys suggest that currently both industrial and academic communities believe that physics-based modelling will continue to be crucial, even while the component of ML/AI in modelling increases. At the same time, it is recognised that with increasing access to data, statistical data-driven methods have a good potential to assist physics-based models, or for some applications even replace them. There is indeed an emerging cautious optimism that synergistic approaches constitute a great opportunity for substantial gains in speed and accuracy.

Verification and Validation. It is important to have precise definitions of validation and verification. The following are generally accepted that verification refers to the internal testing of the computer model, its mathematical basis and any related assumptions, whereas validation is more ‘outward facing’ toward the real-world problems the model is created to investigate. Although there are many model approaches, there is considerable commonality. In particular, a recurring theme is that most authors consider an ideal case in that the model application is well defined and there is an assumption of freely shared information between modellers and experimenters, sometimes including pre-testing to determine related experiments. This is an important factor in ensuring that the model is not used outside the range of validity of its original conception. This is a very well-developed approach, and formal V&V processes have been established, albeit predominantly for continuum models. It is an important process, especially relevant to Integrated Computational Materials Engineering (ICME) where the applications and models are well developed. This is not the case for discrete models. Here, V&V is at an early stage and UQ is a challenging problem. As a result, the formal structures available for continuum models do not exist. Such protocols, allowing a realistic model credibility assessment are urgently needed.

Modelling materials properties at the electronic level has been industrially successful in specific cases, e.g. in catalysis, and in electronic, optical, and magnetic materials. However, many industrially important problems such as modelling thermomechanical and electrochemical properties and processes cannot be solved on the electronic level alone, even if massive computing power were brought to bear. Solving these problems requires first and foremost sophisticated multi-physics and multi-scale modelling. In such coupling and linking (C&L) workflows, models of a lower granularity benefit from information available at an underlying more fine-grained level. Even though the latter approach appears promising the computational demand, the current state-of-the-art is still quite far away from a widespread adoption of this approach. Generating engineering solutions for identified challenges still depends too much on specific toolboxes and it includes equal emphasis on empiricism (namely data-driven). Hence C&L workflows cannot be considered as a stand-alone solution but must be integrated with properly curated data. This is needed in order to move forward beyond "the hype" of big data, IOT, ML, AI and to understand what these techniques really offer as additional toolbox / disruptive changes towards advanced digitalization of materials discovery. Another point emerging by looking at the current state-of-the-art is the maturity of continuum and discrete models on their own. Adopting C&L methodologies to bridge both domains is promising but it is feasible if and only if both advancements with each domain are equally supported. C&L workflows require frequently to reformulate the assumptions at the basis of each domain. Hence C&L development cannot proceed with equal emphasis on the development of continuum models and discrete models.

Analysing the state-of-the-art of C&L, it is clear that we are still far away from the capability to predict aging and lifetime predictions of materials. Methods and tools for lifetime prediction and degradation patterns would be essential for all processes involving wear and corrosion, current and future battery chemistries, materials for the electrolysis of H_2O or CO_2, materials for power electronics, switch gear and next generation power trains, composites/plastics and additive manufacturing materials.

2.1.3 Gaps

Lack of sufficiently good models, leading to lack of trust in modelling

Advancement and improvement of the individual e, a, m, or c models is needed. Force-field development is a crucial example of this type. There are ways to improve the availability of adequate models such as combining them using coupling and linking protocols to reach over larger time- and length scales in the simulations or to take in assistance from data-driven approaches to enhance or even replace some physics-based models. However, the latter two approaches are not yet mature and much development work is needed.

Communication gap

The communication gap between different modelling communities can be a large barrier towards making best use of available modelling tools and human capacity. The underlying origins can be many: different objectives with the modelling efforts, intellectual property barriers, and a knowledge gap due to lack of (access to) personnel trained in modelling.

Gaps in the approach to achieve Verification and Validation procedures

Although V&V works well in specific cases, especially in the context of ICME, the uptake of advanced models by industry requires more general guidelines related to the formal development of convincing model validation to provide the required confidence for potential users. In terms of UQ, tightening procedures to give more reliable comparison with experiment would help to strengthen the V&V process. UQ is still far from trivial for discrete modelling, particularly for atomistic and mesoscopic modelling. However, the formal requirement of credibility assessment procedures within the V&V process demands that robust UQ procedures be developed for discrete models.

A further V&V gap

A further V&V gap relates to systematic errors in a code. As an example, in the area of discrete models, Density Functional Theory (DFT) based models are reliant on approximations to the exchange correlation functional which introduces systematic errors into the model calculations. This is especially important for the calculation of low-lying features on the energy surface. Clearly this can give rise to systematic errors in high throughput searches for new materials using AI and machine learning (ML) techniques. This needs to be systematically investigated and included in V&V+UQ guidelines and is an important challenge triggered by the rapid emergence and adoption of AI and ML in materials modelling.

The feedback collected during the EMMC activities towards the identification of model gaps and the enhancement of industrial uptake of materials modelling led to the identification of particularly relevant challenges, needing priority with regards to materials modelling. The following list concerns gaps that can be cured with improvements within an individual model class, others might be helped by coupling and linking approaches (cf. Section 5.1.3). The list below merely shows some exemplars of the nature of the model gaps that have been raised in the course of the EMMC events.

For example, in the *heterogeneous catalysis* area, there is a strong gap in the availability of adequate reactive force-fields. In the *solid-state microelectronics* field surface effects, defects (often the main source of highly-added value in materials), interfaces, grain boundaries constitute very challenging problems. For *interfaces*, e.g. functional materials, energy materials, composites, for example the effects of defects, surface chemistry, grain boundaries and perhaps additional solvation are all extremely challenging for current modelling approaches to treat. In the *polymer* field there are severe time and length scale limitations for molecular dynamics simulations and robust upscaling methods for macro-molecules are lacking. Reliable descriptors regarding physicochemical properties and inter-particle interactions are lacking, for example in the area of *pharmaceutical manufacturing & nano-safety*.

Major feedback from the EMMC events confirm that the “discrete models” are still at an early stage of industrial exploitation and thus more effort should be put into its promotion and development; however, discrete-to-continuum coupling has the potential to serve as powerful tool in a number of industrial applications and should be promoted. Moreover, efforts should, for example, be made concerning the development of atomistic force-field from electronic calculations, especially reactive ones, exploiting the emerging power of machine learning algorithms. As emerged during the reported events and discussed during the related sessions, the emerging field of machine learning, together with high-throughput simulations, big data mining and automation of the experimental procedures for e.g. high-throughput experimental screening and validation, in line with the migration to Industry 4.0 is believed to have potential to open up new opportunities. However, there also appears to be a consensus in the modelling community (not least among the industrial stakeholders) that the physics-based models will continue to be indispensable.

2.1.4 Definition of success

- While it is important and often helpful to have estimates of the uncertainties of modelling results, the most important is simply that industry has access to models and workflows with better accuracy than what is currently available. This is particularly urgent for complex, realistic systems. Achieving such goals would mark real milestones towards success.
- A long-term funding scheme in place recognising the need for such model/workflow developments in a long-term perspective
- Better understanding of pros and cons in the physics-based and data-driven modelling communities
- Efficient and easy-to-use combined workflows
- Documented V&V framework for discrete models
- V&V applications deployed on European Materials Modelling Marketplaces
- Training activities for early stage and experienced researchers
- Formalised standards (e.g. ISO)
- Review of practical V&V
- Improvement in UQ for discrete models and reduction of systematic errors through improved physical basis of discrete models.

2.1.5 Recommended Action

Accuracy and reliability for complex industrial scenarios

For a wide range of materials properties and processes, current limitations in model accuracy hamper the use of modelling in industry. This concerns the individual stand-alone electronic, atomistic, mesoscale and continuum models, but also *coupled & linked (e.g. multiscale)* workflows. There is a need to (1) push the boundaries of materials modelling closer to realistic, i.e. more complex and large-scale, applications and, simultaneously, (2) ascertain that the models become more accurate than today. We recommend that a long-term funding scheme be set in place in support of such model/workflow developments in a long-term perspective.

Within this action we also recommend an action to explore the synergies between physics-based and data-driven modelling further. Among the actions suggested: collect success stories of approaches that achieve such synergies; make an inventory of ML methods applicable in materials science and design and classify the methods (preferably using an ontology) and start a program to promote them; educate the various modelling communities in new opportunities (potentials and pitfalls).

Enhanced verification and validation procedures

A dedicated V&V+UQ training program for materials modelling should be developed and deployed. One viable model for this process is that established by NAFEMS (International Association for the Engineering Modelling, Analysis and Simulation Community), and here a pragmatic approach could be training on V&V + UQ for academic and industrial model developers, materials modelling PhD students aiming for industrial careers, and specific V&V training for translators.

Furthermore, in terms of UQ, tightening procedures to give more reliable comparison with experiment would help to strengthen the V&V process. UQ is still far from trivial for discrete modelling, particularly for atomistic and mesoscopic modelling. Establishing and strengthening collaborations with the mathematics community are recommended to tackle these issues.

2.2 Interoperability and integration

We define interoperability as the ability of two or more systems to exchange information between them through a common representational system to perform a complex work that cannot be done by each single system alone. The presence of a common representation system provides the highest level of generalization and replaceability and means that no privileged one-to-one connection between two system types should be implemented within the interfaces (see Figure 1a). In principle, in a full interoperability scenario, one system can ignore the details about other systems.

Interoperability stands in contrast to compatibility which denotes the ability of two or more systems to establish a one-to-one connection between them, which is usually due to strong similarities in their internal representations that facilitate mutual understanding (e.g. for software this usually happens when systems are parts of a set of tools provided by a common developer) (see Figure 1b). In a compatibility scenario, systems are fully aware of the type and identity of the other connected systems.

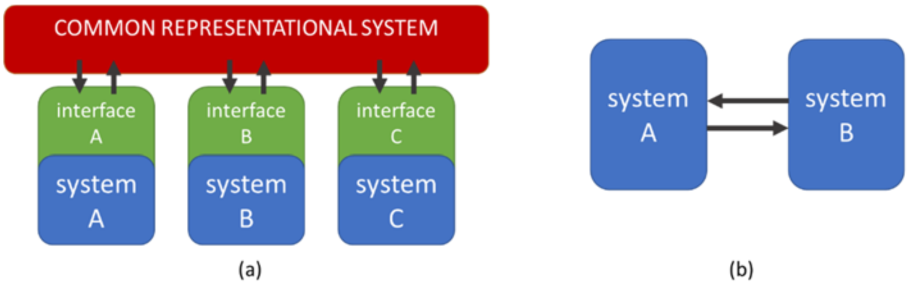

Figure 1: Interoperability (a) vs. compatibility (b)

Integration and interoperability are sometimes used interchangeably. Here we use integration more in the context of the technical integration, i.e. the interfaces and arrows shown in Figure 1. Interoperability enables a more efficient and generic integration by treating each system independently toward the common representation.

2.2.1 Industrial Need

In Industrial R&D, there is an increasing integration of people/communities and insights from different domains and sub-disciplines in complex workflows in order to increase efficiency and effectiveness in tackling complex R&D challenges.

Translating these challenges efficiently into digital workflows requires high levels of interoperability and integration. For example, simulations involving the use of several materials models combined in a common workflow requires orchestrating the interplay of different models, the corresponding software and their data management tools.

These scenarios play out in the context of a drive towards a more integrated and digitalised work environment, in R&D and the enterprise as a whole, leading to the demand for stronger interoperability and easier mining of data across all types of data source, be it modelling or experiment, R&D or business related.

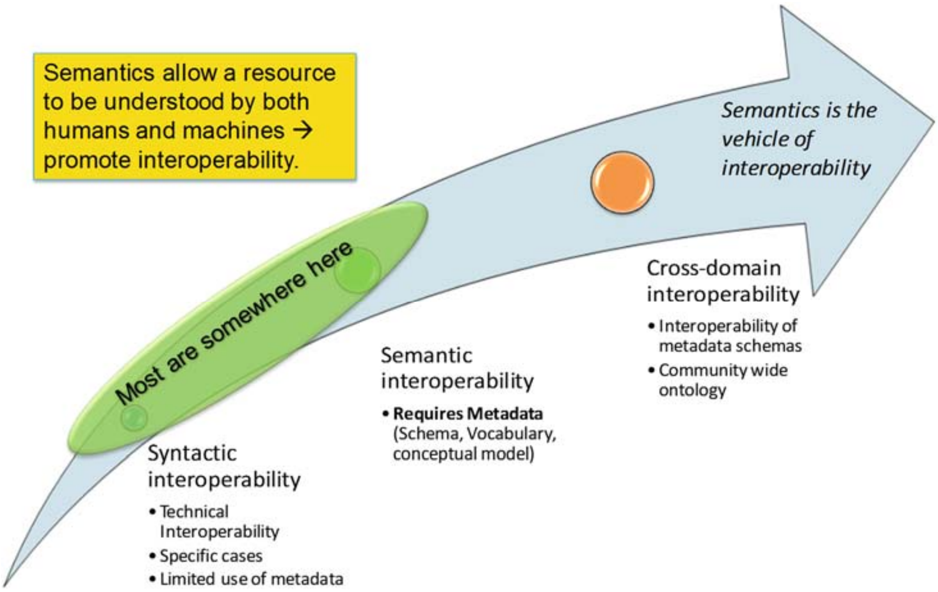

Figure 2: Levels of Interoperability

In order to achieve the vision of “Materials and Manufacturing 4.0”, industry and its value chain require the ability to connect data and models seamlessly and transparently, enabling much faster and more agile integration of new or alternative models into existing workflows and moving from newly designed workflows (e.g. by Translators) to executable solutions much faster. Furthermore, there is a need to utilise modelling assets more widely, to involve a wider range of actors and integrate modelling and data produced from modelling more efficiently in decision making processes. Industry 4.0 requires systematic knowledge integration, hence there is a need for physics-based models, data-based models, lab data and literature data to be more easily reached and processed. It will promote efficient and fast decision making, initially through decision-support guided by experts but gradually also for autonomous decisions, e.g. by manufacturing lines reacting to changing process conditions or materials behaviour.

2.2.2 State of the Art

Today, most integration solutions in materials modelling operate at the syntactic level (see **Fehler! Verweisquelle konnte nicht gefunden werden.**), enabling compatibility between certain codes. It means that integration is often done by import and export of data based on pre-defined formats.

There are exceptions within certain domains where some level of interoperability has been achieved based on domain agreed vocabularies and formats. A leading example is the field of crystallography which has established the Crystallographic Information File (CIF) as an exchange format backed up by widely agreed vocabularies. It is used in a range of modelling environments as well as databases.

The electronic structure and atomistic modelling community has been advancing metadata and schema through a number of initiatives (some involving experimentalists). In particular, the "Open Databases Integration for Materials Design (OPTiMaDe)" consortium has been developing interoperability tools to make materials databases interoperable.

The Open API standard has proven to be a successful way to document REST APIs, allowing easier and more flexible integration of codes, and for developing, managing and executing workflows. There are several open and proprietary integration and interoperability environments which however typically specialise in certain model types.

The quick support and endorsement of the FAIR data principles is an important step towards improving the findability, accessibility, interoperability and reusability of scientific data and other digital assets. These principles emphasise machine actionability, but so far, there are not many systems that fully implement them.

Another important step towards facilitating interoperability for Physics based models has been taken with the CEN standardisation Workshop Agreement (CWA) on Terminology, Classification and Metadata for Materials Modelling. Based on the Review of Materials Modelling[2] (which itself is based on the analysis of well over 100 FP7 and H2020 projects over many years), the CWA provides (a) concise definitions for the key high level terms in materials modelling, (b) a classification of physics based models (by entity, then Physics Equation and subsequently Materials Relation) and (c) a standardised documentation of all aspects of simulations, covering the user case, model, computational representation and post-processing.

It provides the basis for further development of a solid semantic foundation for materials modelling. Other fields of science and technology, e.g. genomics and bioinformatics have made great strides organising their knowledge and enabling collaboration across a wide range of stakeholders by developing such a semantic foundation in the shape of ontologies. An ontology is a formal naming and definition of the types, properties, and interrelationships of the entities that really or fundamentally exist for a particular domain.[c] Ontologies aim to define which entities, provided with their associated semantics, are necessary for knowledge representation in a given context.[3] Ontologies and related information technology provide an opportunity to share a common understanding of the structure of information within a specific domain, the possibility to reuse domain knowledge, to make domain assumptions explicit and to analyse domain knowledge.[4]

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

- A description of materials from a rigorous physics perspective
- Formal relations between granularity levels to facilitate multiscale materials description

---

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

- Definition of material processes to capture the changing and evolution of materials as chain of different states

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

2.2.3 Gaps

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

In particular, coupling and linking (C&L) materials models require standardised ways to describe a use case, including the materials and processes to be investigated, their respective properties, the models and computational representations used. Migration towards standardisation is seen as a pivotal point in the framework of C&L methods. It is particularly important in view of the undergoing development of open simulation platforms and marketplaces. In this sense, having a detailed underlying framework such as a widely agreed ontology will be an added value for interoperability.

Current solutions have been developed with a wide range of different objectives and they lack a common basis in the semantics of materials modelling. The tasks for the materials scientist requiring to go across typical domain boundaries can be laborious and error prone.

There is no systematic approach; each workflow is different: e.g. based on either a simple approach (parameter passing and surrogate models) or transferring, manipulating complex data files.

There is no semantic framework in place. Integration is done e.g. on the programming API level or with manually developed translating files; JSON APIs translations in C++. Such specific solutions can be very efficient, but they are not general. APIs avoid the need to make any change in the simulation software tools to be added to the interoperability environment, which allows an easy extension to new applications. However, the interoperability remains on a syntactic level. This means that it relies on particular metadata (e.g. HDF-based) as common interchange format. No semantic information is yet included in the implementation.

2.2.4 Definition of success

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

- Putting an EMMO based semantic framework and OSP at the heart of Marketplaces, Open Translation Environments and Business Decision Support Systems.

And as a result:

- Ability to integrate new codes faster
- Digitalisation solutions that integrate models and data in a transparent and efficient manner, supporting complex and varied industrial workflows.

2.2.5 Recommended Action

Further development and governance of EMMO for a wide range of materials domains

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

Support development of tools for development and use of ontologies and realisation of the FAIR data principles

Ontologies are not a means in themselves and require a wide range of tools to support communication between models and to verify integration (in low-level, programming and high level, semantics of variables, constraints and phenomena), use by translators etc. This should be done by establishing tools facilitating building and using ontologies, like advanced ontology-based search or ontology-based generation of domain or application-specific metadata. Tools supporting data documentation and easy-to-use libraries and APIs that applications can use to realise FAIR data principles should also be provided.

Support the implementation of Open Simulation Platform (OSP)[d] principles in existing and emerging materials modelling platforms.

Simulation platforms based on EMMO will greatly facilitate workflow generation and execution by humans and machines, i.e. by modellers, by translators and in semi-automated systems such as Business Decision Support Systems, Open Translation Environments and Digital Marketplaces.

An OSP facilitates putting all these pieces together in order to carry out a simulation based on semantics, and with definitions/standards that are independent of specific implementations. In particular it should be straight forward to combine physics equations with materials relations and also straight forward to source and read in data for the parameters of those relations for specific materials. Given a simulation ‘plan’ that has been worked out by a Translator to tackle a certain User Case, the

---

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

Modeller should therefore be able to implement the simulation in an efficient and effective manner. The plan and the outcomes of the simulation will be documented with metadata (based on EMMO) in a way to support data mining and analytics as well as enable others to reproduce the simulation, both using the same codes and using different codes implementing the same models. It will hence be straightforward to replace one code by another in a given workflow. Beyond the 'single' user case, the management of complex workflows requiring either machine or human decisions would be supported by such a platform.

Support creation of common standards with domains outside of materials modelling

Harmonisation of ontologies across domains like materials sciences, manufacturing, engineering and biotechnology and establishment of common standards for data documentation will be key to digital integration and contribute to achieving a circular economy.

3 Making modelling readily accessible ("Framework")

3.1 Data repositories and Marketplaces: Materials Knowledge and Information Management

3.1.1 Industrial Need

Industry expressed needs to access a very wide range of information and knowledge sources in order to support accelerated materials and product development. These range from supply chain considerations, choice of raw materials, composition and combination of materials with respect to properties and key performance indicators all the way to the integration into products.

The choice of materials and composition is a critical step, it requires extensive integrated materials modelling drawing on multiple expertise, electronic, atomistic, mesoscopic and continuum models with particular emphasis on multi-model workflows (multiphysics, multiscale) that are able to probe all aspects from raw materials and processes to properties.

Another fundamental need is for materials modelling to support the market-led approach to development meaning going from the KPI and market demands down to predicting and optimisation of processing and materials composition. This requires augmenting traditional materials modelling workflows with machine learning and big data analytics.

Moreover, a holistic approach to product development requires digitalisation platforms that incorporate digital description of materials in virtual lab and production facilities using so called digital twins. It further emphasises the need to mobilise and collate multiple disciplines and expertise together. Digital Marketplaces should enable industry, and especially SMEs to find, activate and mobilise needed expertise and resources quickly and seamlessly by accessing a network of interconnected sources. With the establishment of marketplace and digital hubs each focusing on different aspects of materials development, industry needs these services to be interoperable and for data repositories be become an integral part of digitalisation hubs and related activities.

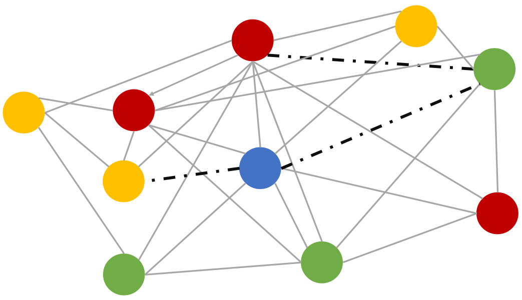

Figure 3: Envisioned web of hubs, a virtual interconnected set of materials development marketplaces addressing various aspects along the development, design, and manufacturing cycle of new products. Dots can stand for various marketplaces from materials modelling to product prototyping and manufacturing. The dot-dashed line demonstrated a cycle containing e.g., materials modelling for design and materials selection (red), prototyping marketplace (green), supply chain set up (blue) and manufacturing (yellow).

3.1.2 State of the Art

Today, there are disconnected digital hubs that are emerging in multiple fields providing only partial support for the entire development cycle of materials. These include two European Materials Modelling Marketplace projects, VIMMP (www.vimmp.eu) and MarketPlace (www.the-marketplace-project.eu), a number of Marketplace like actions, such as within DT-NMBP-20-2018 - A digital 'plug and produce' online equipment platform for manufacturing (IA) (http://market40.eu/, http://www.weldgalaxy.eu/about-weldgalaxy/), characterization open innovation environments (OYSTER, MMAMA, CORNET projects), innovation hubs of DG CNECT (MAX, NOMAD) as well as commercial platform providers (such as https://3dexperience.3ds.com/3dexperience-marketplace/, and https://matmatch.com/), international actions such as www.Nanohub.org in the US, KiRI (KIST R&D Informatics) from Korea (http://kiri-home.kist.re.kr), and NIMS Nanotechnology platform in Japan (https://www.nims.go.jp/eng/infrastructure/nims_nanotechnology platform.html),

3.1.3 Gaps

Each marketplace and marketplace like platform focus on specific sectors and such offers only part of the needed materials development needs. While materials modelling marketplaces aim to provide complete modelling needs for SMEs and industry in general, there is a gap between the demands of industry with respect to covering the entire development cycle. In addition, there is a lack of demonstration of how materials modelling marketplaces can be used in practical development questions. Most actions are still not interoperable and it is hard to combine in a complete cycle due to lack of interoperability mechanisms.

3.1.4 Definition of success

The ability for end users from industry to link services horizontally across vertical marketplaces and address the entire materials development cycle (see Figure 4) will affect industry in a profound way. The desire to create a digital twin of materials and perform various actions on it in different thematic hubs is highly demanded and will ensure continuity in development efforts, and boost efforts of entire industry sectors.

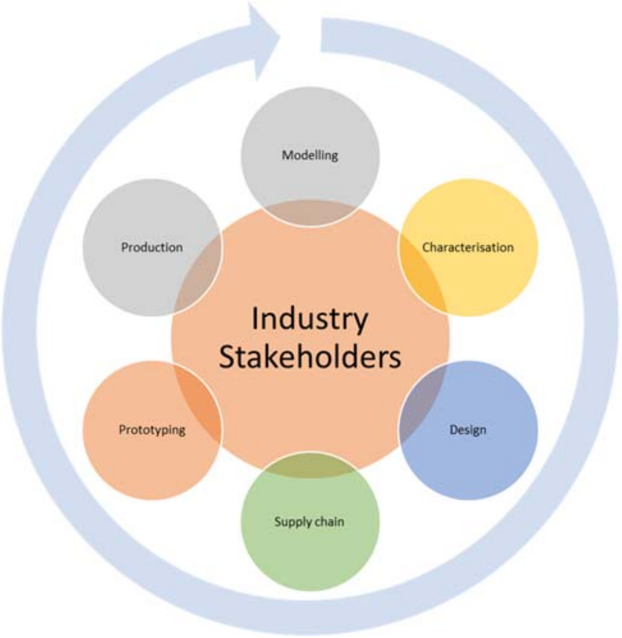

Figure 4: Interoperability between Marketplace and collaboration platforms enables industry ready and seamless access to the entire development chain. Some examples of platforms being developed in EU actions are shown (list is not exhaustive).

3.1.5 Recommended Action

The goal is to link and network existing and emerging platforms and in particular create a holistic global digitalisation network of hubs (see Figure 3). Actions to boost interoperability, enabling the transfer of information from one hub to the other by information owners (and hence comply better with DSM and GDPR) as well as the ability to combine various services from across all components contributing to materials and product development. There is a need for the following actions:

1. Coordinate and network various existing digitalisation and collaboration marketplaces and marketplace like actions.
2. Engage actions for boosting and developing interoperability between marketplaces in various domains. These actions should be part of ongoing materials development efforts and not limited to materials modelling only.
3. Engage in vertical actions to develop needed thematic topics for digitalisation platforms and hubs spanning all aspects of materials investigation and with a focus on domains contributing to the Green Deal (e.g. energy, lightweight materials, sustainability and environmentally low footprint materials for all application fields).
4. Engage in actions for developing digital twins in the widest sense including materials modelling based twins and linking to prototyping and manufacturing actions.
5. Engage in actions for creating horizontal digital hubs by standardising on common interfaces and user management in tandem with coming ontology projects.
6. Actions to create demonstration or prototypes of entire innovation cases from conception of an idea to a product implemented on various available digitalisation hubs and marketplaces.

3.2 Translation and Training for Companies

Translators are individuals with the necessary competences to translate industrial problems into modelling activities and simulation protocols. These stakeholders promote innovation, creating new opportunities from the bottlenecks and problems limiting industrial development. Their activity requires promoting collaboration among the different stakeholders involved in materials modelling activities, namely industrial end users, software owners and academic model developers. Thus, they possess a multiplicity of skills, spanning technical modelling background, economic concepts and soft skills, which are combined to enhance collaboration among different stakeholders to the benefit of innovation. Clearly, this role implies strong communication abilities, which are essential to bridge the "language gap" among the different stakeholders. Today, people with these skills may work as academics, software owners/engineers, independent consultants or modelling experts inside a (usually large) company.

3.2.1 Industrial Need

Modelling is widely applied in industry as a useful tool to provide insights and develop improved materials, products, processes. However, often the full potential and benefits of modelling are not fully explored by industry, either due to limited modelling expertise inside the company or a lack of awareness of what is available and possible. Therefore, there is an industrial need for partners who are able to translate innovation challenges into modelling solutions and provide guidance, training and support in implementing the modelling solutions inside the company.

The industrial need for translation depends on several factors such as the level of internal modelling expertise/knowledge of the company, its size, position in the value chain (e.g. material producer or product manufacturer/converter), domain of application/market (e.g. automotive, pharmaceutical). The industry needs and also expects from the Translators that they understand very well their business case and technical challenge, to conform to confidentiality (when requested) and to offer to the client in an objective and well-grounded way the most beneficial/useful modelling solution for the specific industrial case.

The importance of such experts has strongly emerged as an effective means to accelerate industrial innovation, which also motivates the definition of a clear and well-defined strategy for their training.

3.2.2 State of the Art

As a result of EMMC activities, the role of Translator has been defined and is now widely recognised. EMMC has in particular focussed on: (1) regulation of the role and tasks of the Translators (in line with their expected activity in the segment of industrial innovation); (2) identification of training requirements and definition of proper training protocols; (3) collection, analysis and distribution of (publicly sharable, non-confidential) case studies.

With regards to the first point (1), the most important outcome has been the Translators Guide[5], which contains all the most relevant aspects related to their activities and obligations. These include specific guidelines and features according to the different types of Translators that may be identified (e.g. internal/external Translators respectively for big companies and SMEs). The Translators Guide is intended to be used by Translators themselves for guidance and also by the industrial end users to know what to expect from Translators.

With regards to their training (2), extensive work has been dedicated to the identification of the most important concepts in line with the Translation Guide (required skills). Given that these professionals often present a technical background, particular effort has been dedicated to the identification of the economic aspects of their training requirement. This has allowed to clarify some of the most critical aspects that a "Training for Translators" course should encompass, namely e.g. management of innovation, budgeting, intellectual property, etc. All the available information and training materials has been made publicly available to the newly established Translators network in the form of (short) video courses (to be found at https://www.youtube.com/c/european-materials-modelling-council).

Along with these introductory video courses, various Translation cases have been collected and the public ones made available on the EMMC website (3). These cases contribute to making material models more accessible and usable by highlighting the benefits for companies of using material models to solve specific industrial problems. The translation cases also show how the company found the Translator supporting the idea to make Translators and models more easily accessible to the companies. These cases represent examples of solutions (performed by different types of Translators and for different types of industrial clients) that may inspire other clients with similar problems and can be used as a reference and for (training) best practising by the Translators.

All these activities led to a wider recognition of the translation process and of the Translator role, not only by industry but also by institutions and individuals with an interest (and potential skills) to be translators.

3.2.3 Gaps

The main gaps which remain to be addressed are:

1. The business model for translation is not yet (fully) established. Translators (or institutions such as academic organisations and software companies) and manufacturing industry should be further stimulated to adopt/implement translation in their practices.
2. How would Translators and their role fit into the ongoing digitalization of the EU industry? For example, considering the transition of industrial innovation towards (big) data and related mining, would training of Translators include concepts about artificial intelligence? Specific considerations about this point may lead to a refinement of the training protocol for Translators and eventually include fresh concepts about big data and their mining via artificial intelligence.
3. Clearly identify how Translators relate to the ongoing development with online Marketplaces for materials modelling, e.g. how would Translation services be offered and digitally integrated into Marketplaces?

3.2.4 Definition of success

Successful (further) establishment of the role of the Translators as key players for EU industry should consider the following aspects:

- Improve the database of case studies, for best practices and continuous education of Translators. This database should be enriched, particularly with cases for SMEs, and eventually related to Marketplaces in the form of cases/training sections.
- The role of the Translators over the next few years must evolve as industry is moving more and more towards data-driven innovation.
- Open Translation Environments should be established for access and for exchange of translation practices and data between translators.
- Digitally integrated Translation services on Market Places.

3.2.5 Recommended Action

1. Special attention needs to be paid to translation for SMEs: e.g. the (modelling) tools need to have a certain level of maturity, new models and approaches may generate too high (economical) risk for SMEs, establishing new arenas of cooperation and guest periods/internships. Outline business model(s) for translators that can encourage more institutions/individuals to become or to position themselves as translators.
2. To prepare Translator to consider data-driven modelling in combination with physics-based modelling when proposing modelling solutions for the industrial problems
3. To stimulate academic institutions to recognise and to invest in employees who perform the translator role, e.g. via creating a team of experts possessing the wide range of translators' skills or via training academics to become professional translators (as part of their regular tasks) including offering teaching courses to students to be trained for the role of the translator.
4. More opportunities for training courses and programs may be considered, as well as a formalization of a career at the university level.
5. In perspective, additional concepts regarding machine learning in the context of Translation may be considered as a further opportunity to extend knowledge and effectiveness of Translation in the context of data-based innovation of the European industry.
6. Translators need to prepare themselves to enter and offer their services on the Marketplaces, e.g. via preparing and sharing translation cases to build expertise and trust. Engagement is desirable with the two H2020 materials modelling Marketplace projects to facilitate/support the implementation and the establishment of translation on the platforms they are developing.
7. Make Translators and industry aware of the translation platforms (open translation environment or/and Marketplaces), when they are ready to use, via dissemination means and via continuing collection of translation practices/cases.

3.3 Industrial Software Deployment

3.3.1 Industrial Need

European manufacturing industry is driven to high-value-added products and highly sophisticated processes as commodities have moved to low-cost countries. This makes materials modelling particularly challenging due to the complexity of the current industrial problems involved.

In this highly competitive global market, industrial decision makers need to see a clear benefit of materials modelling in the form of success stories. With time to solution being essential, industrial engineers and scientists need reliable, validated, and comprehensive materials modelling software. Professional long-term maintenance is critical for industrial deployment since the lifetime of materials modelling software is measured in decades. Responsive support is another critical factor since the major value for companies is the time of their employees.

In order to widen the use and impact of materials modelling in industry, in addition to the above discussed “content” and “framework” requirements, industry needs easy-to-use and well supported software that can be readily deployed and integrated into existing R&D infrastructures.

In several EMMC expert meetings it was pointed out that dealing with complexity is more important than highest possible accuracy. Often, rapid answers (i.e. within a few days or weeks) are needed. This is particularly important for SME’s, while R&D departments of large industrial organizations may have the ability to work on longer timescales and on more fundamental issues.

3.3.2 State of the Art

The current state of the art in computational materials modelling is characterised by outstanding achievements especially of European university groups developing modelling software. Due to decades of dedicated academic efforts Europe has gained global leadership in academic materials modelling software for condensed matter including the simulation of systems such as catalysts as well as soft matter systems.

However, deployment of discrete materials modelling software in European industry remains limited to a relatively small number of about 30-35 companies. It is mostly found in the R&D departments of large industrial organizations in the chemicals industry and has been introduced in other European industries such as the automotive and aerospace sectors only recently. This is in sharp contrast to the situation in Japan, where the leading automotive companies have been using electronic structure calculations and atomistic simulations for over three decades. It has been noted in the 2nd International EMMC Workshop in 2019 that “the European automotive industry is catching up”. To a large extent, this is driven by the urgent need for improved materials for batteries and fuel cells. In this area, Japan and South Korea are in a strong position, China is pushing very hard, thus challenging the US and Europe as well as Japan and South Korea.

Driven by “big data” and “machine learning”, there is great excitement, if not to say hype, to replace theoretical-computational approaches based on first principles by data-driven research and development. From a number of comments made in various EMMC workshops and expert meetings, it is clear that a wise combination of physics-based and data-driven R&D is the proper way forward.

Overall, it is fair to say that the current state of the art in material modelling is still to a large extent academically driven, focusing on the development of novel methods (e.g. machine learning interatomic potentials) and ground-breaking applications published in high-impact journals rather than on solving practical industrial problems. As a result, software developed by academic research groups, often brilliant and innovative, is not well aligned with industrial needs.

3.3.3 Gaps

The major gap between academic software and industrial deployment of materials modelling has its root in the fundamentally different objectives and motivations of academic researchers and industrial organizations. Rightfully, academic research is focused on developing and publishing novel concepts, innovative approaches, and revolutionary discoveries (e.g. novel 2D-materials or novel superconductors). Systematic software development, large-scale validation, comprehensive documentation, and especially long-term support are usually not the primary concern of academic researchers. However, since academic developments are often at the origin of innovative software, academic software developers need to be fully aware of issues such as modularity of software, interoperability, intellectual property and implications of license schemes.

On the other hand, industrial R&D organizations are largely driven by the need of adapting existing materials to changing market demands and by optimising the efficiency and environmental responsibility of existing processes. Of course, introduction of completely novel materials and disruptive processes is necessary in a competitive and rapidly changing world, but this is pursued with great caution given the risks involved. In response to these industrial needs, materials modelling software has to help in improving already existing and highly optimised materials and processes while also supporting the development of completely new solutions. Ease of use, high reliability, broad validation, and long-term professional support as well as clear licensing models are essential requirements for successful industrial deployment of software. Thus, there is a fundamental gap between academic software and industrial needs. Software companies can bridge this gap between academic research and sustainable industrial software deployment.

3.3.4 Definition of success

Successful deployment of materials modelling software can be defined by the following criteria:

- Successfully improved or novel industrial materials and processes where materials modelling has played a significant role in their development.
- Patents including materials modelling.
- Industrial investments in staff and equipment related to materials modelling (e.g. size of materials modelling groups in companies) and their persistent growth.
- Successful technology transfer between academic research software and their commercial deployment.
- Global recognition of European leadership in materials modelling science and technology.
- Growing global market share of European software companies and their economic health.

3.3.5 Recommended Actions

1. Foster the synergy between academic research, software companies including technology consultancy, and industrial deployment.
2. Provide guidance to young academic researchers as they develop software components in terms of industrial software requirements, clarity in ownership of software, and license models[6].
3. Increase the mutual understanding of the complementary role of the different stakeholders, namely academic, software companies, and industrial users by coordinating and supporting their communication and interactions. Examples are industrial internships, joint Ph.D. programs, and consultancy arrangements.
4. Raise awareness of software business models[7] and the socio-economic implications of "free" open source software.
5. Support the creation and growth of European materials modelling software companies in terms of innovation grants and tax incentives, fostering continued global leadership of European materials modelling and digitalisation software industry as a cornerstone of manufacturing industry competitiveness.
6. *Scientific software development.* To foresee and plan specific careers in scientific software development. A sustainable model for the development of scientific software is required, since there are currently no careers in the field, and we need to have careers paths for those experts. Possible options to this goal are: Embedding specific careers in existing academic or research institutions; Embedding specific careers in supercomputer centres or national facilities; Embedding specific careers in a distributed model (a virtual Joint Research Centre). Development of scientific software can be fostered by the Commission, asking specific requirements: for example, to be public, verified and validated, and embedded/representing major communities.

4 Creating Industrial Impact ("Implementation")

EMMC has been analysing industrial impact from different perspectives and has already published several reports and White Papers[8,9] on this topic. They provide not only evidence for impact but also the tools industrial R&D requires in order to assess impact mechanisms and develop strategies to enhance R&D productivity by means of improved use of modelling and digitalisation of materials.

In general, there is a need for further development of econometric models and associated data gathering to support an industry transformation towards a model-based approach. However, also more anecdotal evidence is seen as very useful and there is still a need for more success stories that raise the awareness of the potential of materials modelling in terms of technological innovation.

In particular, the multi-facetted nature of impact generation is represented by four 'dimensions', which are Tools, Data, Processes and People[9] . Organisations are encouraged to assess and track their 'maturity' and set targets in each of these dimensions. Furthermore, the materials modelling ecosystem needs to further elaborate its current status, objectives and barriers as well as specific actions to improve the maturity in each of these dimensions, enhancing the industrial impact.

Tools

The Tools dimension includes the physics- as well as data-based models needed in industrial applications, workflows and algorithms, software implementations and methodologies as well as hardware. It also includes coupling and linking, optimisation, uncertainty quantification, verification and validation.

Data

The Data dimension includes data generation, qualification, curation and annotation, storage and mining, as well as related technologies including data schema, taxonomies and ontologies. Furthermore, aspects of data include managing ownership/IP, confidentiality where required, provenance as well as standards.

Process

The Process dimension includes different business processes ranging from specific tasks such as performing a simulation via activities such as modelling and simulation, to higher level processes such as R&D and manufacturing. It also includes (internal and external) collaboration processes. Modelling enters into these in different ways and via different tools and infrastructures. For example, a modelling function is enabled by certain IT processes, an R&D function benefits from well-established translation processes and business processes can integrate modelling via a Business Decision Support System.

People

The People dimension includes the human resources, or workforce and its 'engineering' and talent development. Considerations that fall into this category include not only recruitment and training of highly skilled modelling experts but also translators, training of occasional users, and ways of achieving what is often termed democratisation of modelling.

A maturity self-assessment by industry[e] provides the following picture as shown in Figure 5 (note that maturity levels range from 1 (Initial; lowest level) to 5 (Optimised; highest level)). Industry regards its maturity in the adoption of materials modelling as at medium level or below (typically between levels 2 and 3). Maturity is highest for People and lowest for Data and Process.

---

[e] Collected via a survey by EMMC with participation from 16 companies representing different industry sectors, see Ref [9]

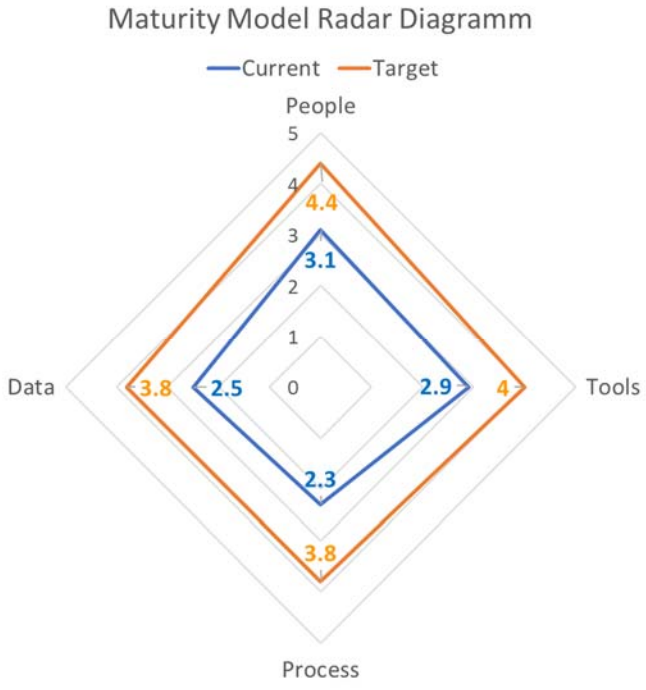

Figure 5: Current (blue ribbon) and target (orange ribbon) of Materials Modelling maturity: Initial (1), Defined (2), Integrated (3), Managed (4), Optimised (5)

Furthermore, there is evidence of a steady long-term growth of maturity in organisations, i.e. organisations with many years of experience typically reach higher maturity as shown in Figure 6.

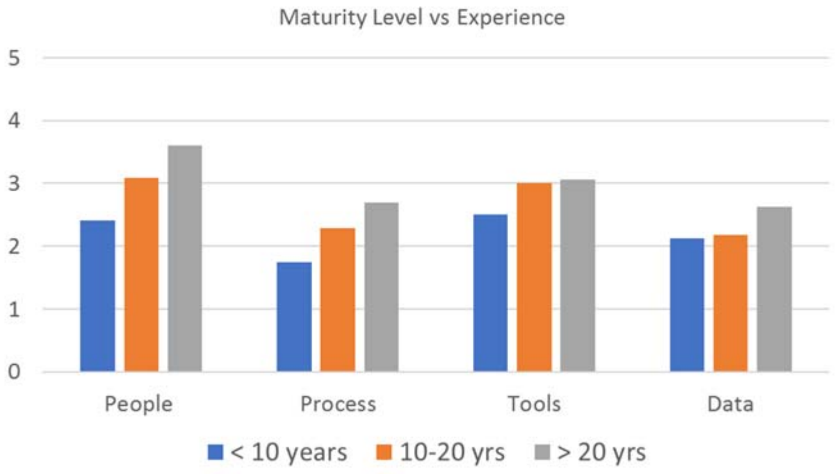

Figure 6: Maturity of the four Dimensions vs years of the organisation using material modelling

Hence, actions are required to achieve wider and more sustained impact of materials modelling at an enterprise level rather than a dependence on ad hoc success stories and individual 'heroes'.

In the following, each of the maturity model dimensions will be discussed.

4.1 Tools

4.1.1 Industrial Need

As was discussed also in Section 4.1, industry requires better verified and validated as well as integrated models that enable multi-scale and/or multi-physics modelling. While advancing the accuracy and maturity of models depends on a range of actors, industry considers the lack of knowledge of accuracy and lack of validation as key barriers.

Regarding software, while industry has well established access e.g. to the latest version of software that a company licenses, there is a need for easier access to information and knowledge about the wide range of existing and emerging models and software tools on the market.

Hardware access and use is likewise well established in larger industrial organisations. However, organisations that have started modelling more recently and SMEs may struggle with deploying hardware and hence there is a need for easier access and potentially SaaS solutions that lower the entry barrier.

4.1.2 State of the Art

The State of the Art in terms of the application and impact of modelling has been documented in a wide range of case studies, a number of which are available as EMMC resources. The EMMC Maturity Survey showed (Figure 7) the highest maturity levels regarding being up to date with the latest versions of the software, the availability of adequate hardware and the expert knowledge of the materials modelling software tools. On the other hand, organisations gave a lower rating to the model maturity (e.g. regarding knowledge and control of model accuracy, degree of validation), the usage of multiscale modelling and the **integration of** modelling software well integrated with your other tools (other modelling tools, LIMS, ELN, enterprise platforms, business decision systems, etc.)

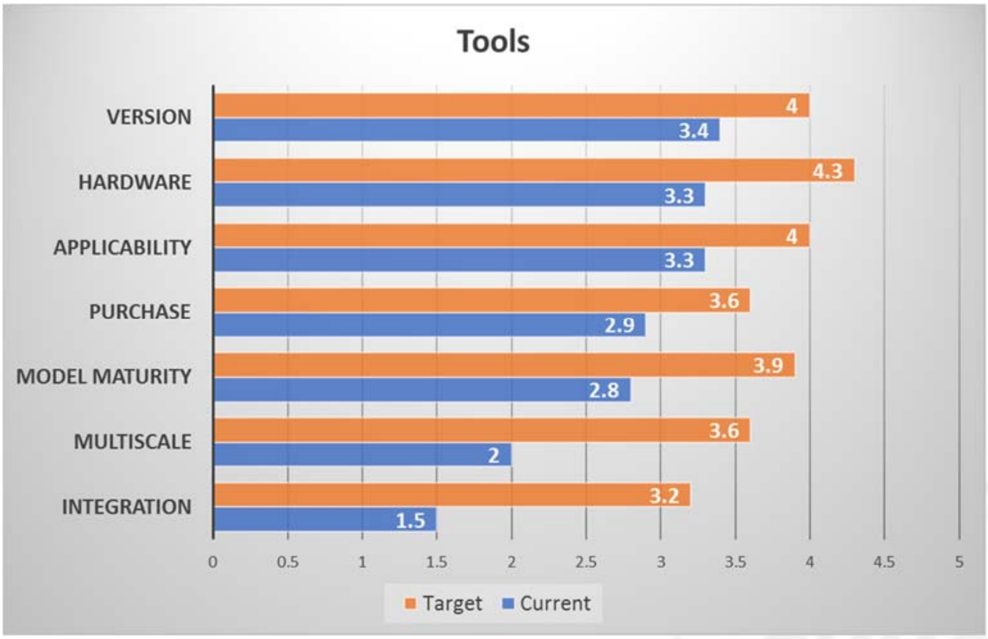

Figure 7: Detailed maturity levels of the Tool Dimension

4.1.3 Gaps

As can be seen in Figure 7, the biggest maturity growth is sought the better integration and multiscale modelling, followed by the maturity of models used and better hardware access.

4.1.4 Definition of success

- Concerning model integration and maturity, a definition of success will be the adoption of materials models, in particular discrete models into the industrial practice, in all stages of development of novel materials.
- Concerning 'multiscale', coupling & linking methodologies must prove to provide an added value with regards to standard approaches. Coupling & linking models and interoperability development, *per se*, are pointless, if they are not guided towards a reachable industrial target, beyond existing standard approaches.

4.1.5 Recommended action

With regards to the identified general bottlenecks discussed above, the following points need attention and may be considered as policy/funding recommendations:

- Make available (open) databases of successful case studies and application of model integration and Coupling and Linking methods in industry, which have emerged as a critical point to increase the confidence on the adoption and use of these methods in industry.
- *Model(ling) accuracy and reproducibility*. To promote integration of materials modelling with equipment and experimental facilities (e.g. robots, high-throughput synthesis, measurements and characterization) in line with Industry 4.0 and towards better and more reliable models. Systematization of the procedures for verification and validation of models as well as procedure for uncertainty quantification (UQ), particularly critical in C&L methods due to the propagation of error through multiple models. Also, we need to understand how to deal with heterogeneous low-quality and high-quality data and to use outputs of models for improving the quality of experimental data, for reducing the heterogeneity of data, for integrating data coming from different sources.
- Only a well verified and validated model can deliver a reliable ROI, hence industry is also called upon to collaborate and invest more in this area, for example by agreeing on "benchmark" validation tests similar to those widely used in engineering simulations. Support a verification strategy of material and process models by a formal body, including benchmark use cases.
  Mirror the current initiatives in the area of continuum and micro-scale modelling (e.g. CMH17, NAFEMS) by addressing the need for benchmark use cases for materials models, and requirements for model quality.
- Agree a combined physical and virtual test programme for a class of materials. Perform Round Robin experiments to test available models using available qualified materials and processes.

4.2 Data generation, qualification and validation

As a general remark, data (-bases) and models share some similarity in their general purpose: Both provide data that are potentially useful to solve some problem, to optimise some product etc. The problem of databases in general is that they might not contain exactly the data being searched for. In case the desired data are available, however, they can be retrieved almost instantaneously. Models in the best case can calculate exactly the data being desired (in future event with a desired accuracy) with the drawback of requiring quite a time and effort to do so.

4.2.1 Industrial Need

There is a need for materials and process information for decision-making at all stages of the R&D process. At the concept stage, less precise information is needed, and yet the materials and process decisions have a significant bearing on the overall costs of the final product (upwards of 80% of product life cycle costs are locked in at this stage). A range of information is used to inform materials/process selection including properties, behaviour and performance, which can be informed by materials modelling with a reasonable degree of accuracy. At this stage, the point of pain is the lack of sufficient physical data to calibrate models for new use cases, or design scenarios.

At the detailed design phase, materials and process qualification are required by regulated industries (e.g. aerospace, medical) on the basis of their continuum (or macro-scale) properties. Qualification programmes are costly (e.g. 1000 to 3000 coupon tests depending on criticality and conditions, as well as sub-to-full-scale testing, references), and risk of time-to-market and failure to achieve qualification is high. Commonly used materials are often tested for a shared database, which reduces costs across supply chains. Materials modelling offers an additional cost and risk leverage by reducing the number of experiments within any given test programme. The point of pain at this stage of the design process is sufficiently verified models to the level of scrutiny and accuracy required by regulated industries, and also appropriately qualified physical test data to both calibrate and validate the models for use in the specific design scenario.

4.2.2 State of the Art

As in other fields, there are huge amounts of structured and unstructured data relating to materials with only a fraction being exploited by now. Materials Modelling is both a source of these data as well as a need for data e.g. for model development, calibration and validation. To be useful and exploitable data must be organised in a FAIR way (Findable, Accessible, Interoperable, Re-useable). This generates a need for data standards, wording standards and nomenclature, where words and their meanings must be understandable by machines.

The EMMC Maturity Survey considered a range of data aspects including the usage and analysis of data from modelling together with data from experiments, awareness of data analytics, data storage solutions, data presentation and data capabilities and practices as well as the combined analysis of data from modelling together with business data sources (customer, suppliers, KPIs, finical forecasts, etc.). The current and targeted maturity levels are shown in Figure 8, strengths in the combination of modelling and experimental data, and relatively lower levels in data sharing, awareness of materials modelling data in the organisation and the use of /integration with business data.

4.2.3 Gaps

There is in particular gaps in a number of the aspects probed by the maturity survey, and in general industry targets a considerable increase in data capabilities in the next few years.

FAIR data from a range of relevant sources, such as physical test programmes are needed for calibration and validation of materials models as well as to organise data determined from simulation using all types of models.

There is a lack of data organisation based on a coherent semantic foundation as discussed in previous sections which is also a barrier to industrial impact.

Figure 8: Detailed maturity levels of the Data Dimension

4.2.4 Definition of success

Based on digitalisation of materials including all knowledge sources in a coherent semantic environment as well as increased awareness and capabilities in data analytics, it should be possible to utilise the most accurate data for a dedicated setting/question within a given timeframe, either via retrieval from databases or by generating them from modelling. The definition of success thus is a question of scope and relates to the degree of accuracy, the degree of similarity (of already existing data), the speed of data generation (by models) or data retrieval (from databases).

The following considerations are important regarding databases.

- Databases can be populated off-line well before the data themselves are needed either by modelling ("pre-calculation strategies") or experimentally (by high-throughput experiments). Databases can be rapidly queried and provide a solution to the dichotomy of speed versus accuracy.
- For the application of materials and process modelling at the early design phase, or for less critical applications, or those informing the behaviour of materials but not linked to qualification/certification, there are harmonised protocols and benchmark physical data which can be used for model calibration and validation. The data quality and level of reproducibility needs to be agreed and updated as the state-of-the-art progresses (both for physical characterization and models).
- For the application of materials and process modelling in critical applications (i.e. models have reached an accepted level of verification), there is an accepted qualification test programme combining virtual and physical test data at the coupon-level for standard materials which are accompanied by sufficient understanding of the behaviour.

- In addition, an accepted equivalency test programme for the manufacturer (material supplier, parts producer) which is enabled by an accepted 'digital twin' of the material and coupon is important. The test programme needs to be statistically robust.

4.2.5 Recommended Action

- Support FAIR data maturity programmes.
- Support integrated materials digitalisation across all disciplines (modelling, characterisation etc.)
- Support increased data analytics skills for industry.
- Develop "pre-calculation" strategies to populate databases, which then can be queried in real time.

4.3 Processes

4.3.1 Industrial Need

In order to remain competitive, industry needs to innovate which in turn requires running an efficient and effective R&D process that itself is integrated well with a number of business process and value chain interactions. While it is widely recognised that digitalisation and a more model-driven approach will impact efficiency, effectiveness and agility, there is a need to identify specific process improvements for industry to target.

4.3.2 State of the Art

The EMMC Maturity Survey (Figure 9) probed the state of the art regarding the tracking o the impact of materials modelling, the utilisation of materials modelling influence in decision making, the use and documentation of translation, how strongly materials modelling features in R&D processes, the degree to which materials modelling contributes to the life cycle phases of products, the extent to which modelling supports product improvements, the use of modelling across the vertical chain from lab to product and the horizontal value chain (supplier, distributor, convertor etc).

Overall Process turned out to be the lowest maturity dimension, in particular for integration of modelling along the value chain as well as from lab to product.

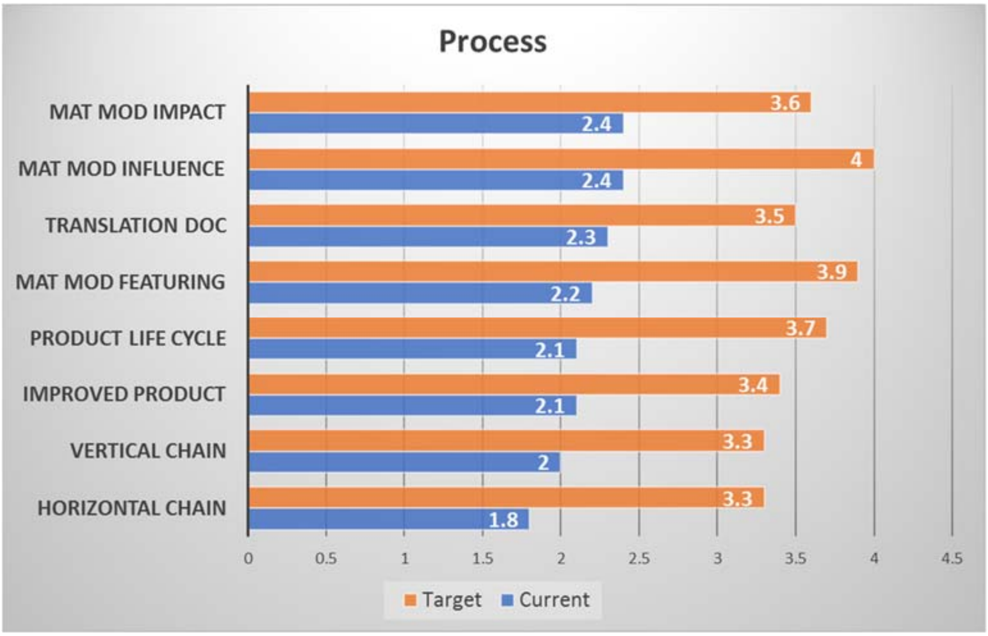

Figure 9: Detailed maturity levels of the Process Dimension

4.3.3 Gaps

The Process dimension needs to grow more than one maturity level in all aspects to satisfy the wished-for targets. The biggest maturity growth is sought for the model featuring in and influencing of decision processes and its role in the product's life cycle and horizontal value chain. Currently, there is a lack of standards which prevents integration of models into R&D workflow for the most impact. In addition, it was identified that collaboration processes between various stakeholders to achieve advanced materials development workflows is limited, to some extend since each area is developed in isolated silos targeting specific vertical application fields.

4.3.4 Definition of success

Vision of success is a much closer integration of modelling into R&D processes at all levels, in fact a model-based digital continuity that R&D staff, manager and the business can work with from different perspectives. This will be integrated materials modelling into the product life-cycle, enable a cradle-to-cradle realisation due to the deep knowledge about all aspects of a product, including the detailed chemistry of materials in a product.

Likewise, materials models are more important in the horizontal value chain across supplier, distributor, convertor, brand owner, consumer, both as a means of exchanging information and as an add-on to a product, a concept sometimes referred to as Product +. Examples include materials relations tuned to the specific materials produced that support manufacturers in the simulation of materials processing[f]. A model-based approach will aid with answering "what-if" questions due to suppliers offering different starting materials and customers demanding different ingredients.

---

[f] See e.g. http://www.performance-materials.basf.us/ultrasim

4.3.5 Recommended Action

Future actions should consider the strong overlap and confluence of modelling and digitalisation in support of making R&D processes more efficient and effective. Modelling includes all physics-based and data-based modelling, and should be closely integrated with characterisation into coherent workflows/processes, for multiple reasons: characterisation is key to model validation, and vice versa, models are required to interpret characterisation data, hence there is a strong synergy. Both are 'as one' when it comes to making R&D more efficient and effective. In the end, both need to flow into a digital continuum that supports workflows, R&D processes and business processes at various levels of the enterprise.

4.4 Workforce Engineering /Talent Development

4.4.1 Industrial Need

Technical expertise vs costs. Using materials modelling requires high-level technical background, which is not always easy to maintain in industry given the cost of such dedicated experts in R&D department. This can only be afforded, in general, in big companies where materials science is a leading business. This is not often the case in small and medium enterprises (SMEs), which may not have the budget for dedicated people for materials modelling and research. These latter may resort to Translators; however, Translators with specific expertise on C&L methods may not be easy to find and their background must be complemented with economic skills.

Data-savvy employees represent one of the largest assets for current and future enterprises, and the absence of simple mathematical or quantitative understandings of reality is one of the most glaring shortcomings of any workforce. Advanced quantitative modelling is, on the other hand, restricted to few very skilled workers, and it can be mission critical. For the first need (broad mathematical skills, gathered on the generic open job market) it seems that countries with a more successful and ambitious schooling program (see below, for state-of-the-art) will have the future largest workforce with general quantitative skills. For the advanced modelling target, one can hope and expect that there will be a very skilled and mobile community, willing to move to countries where the quality of life is high. On these two counts, Europe is in principle well situated.

4.4.2 State of the Art

Communication/interaction gap

Adoption and usage of C&L methods often requires tuning of the input parameters via experimental means. This may represent a limit, as establishing efficient interaction between modellers and experimentalists is not always a straightforward task. Again, here Translators may help; however, their background should be appropriate to interact with experts on C&L methods. This problem arises not only during the first phases of modelling for the input data but also during the validation of the modelling results. Thus, this represents a major issue to circumvent to enhance use of C&L methods.

The EMMC Maturity Survey showed (Figure 10) that the People dimension achieved both the highest current and target maturity with strengths in particular in Collaborations, Recruitment and Continuous Professional Development (CPD) in industry.

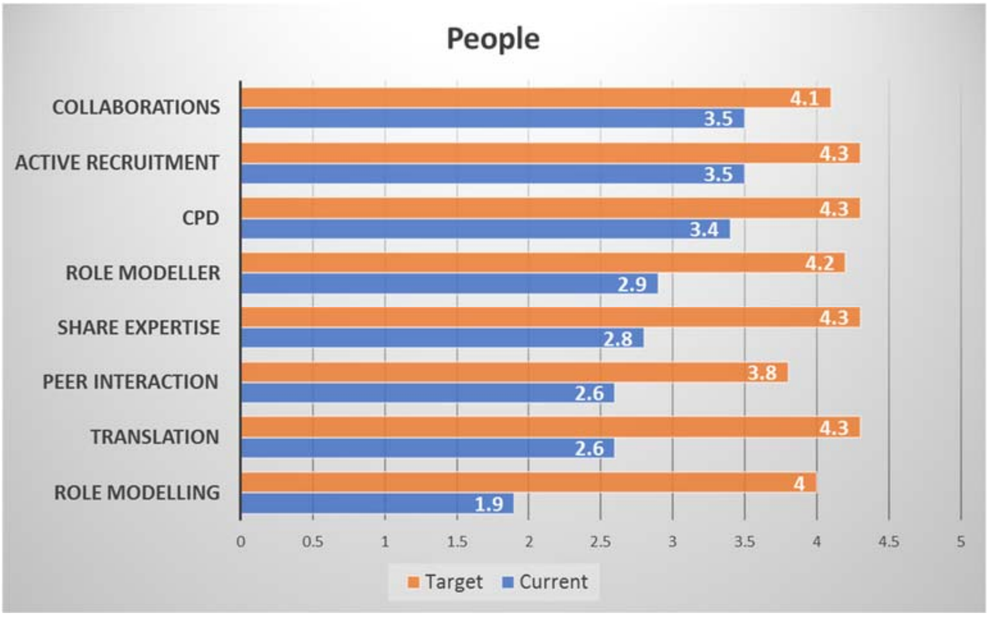

Figure 10: Detailed maturity levels of the People Dimension

4.4.3 Gaps

The biggest gaps were identified in the shared understanding of the role of materials modelling across the organisation as well as in the role of translation.

Despite the relatively low gap, recruitment and CPD were mentioned often mentioned in comments from industry as key barriers in the sense that the materials modelling job typically requires a huge depth of domain knowledge combined with translation/communication skills, hence it is difficult to recruit and train staff. Also, the lack of (continued and sufficiently large) investment was mentioned, i.e. that often there are too few modellers to make a real difference. There is also currently a lack of differentiation in the job role of materials modeller, since “materials modeller” is as wide a description as for example “chemist”.

4.4.4 Definition of success

A nimble and dynamic modelling workforce that is able to evolve in time as novel tools enter into production. The organisation shares a clear understanding of the different roles involved in successful adoption of materials modelling, including the expert modeller, occasional modeller and translator and support their continuous development and integration with other functions.

4.4.5 Recommended Action

- The wide range of roles of materials modelling in industrial organisations require further support, defining and recognising the different roles and their training requirements, and determining the best mix of such roles to maximise the impact in an industrial R&D organisation.
- In particular, Translators can take on the role of ensuring that materials modelling is more easily accessible, better integrated and outcomes are shared more widely in the organisation. Thanks to the capacity to bridge the language gap between the different players in the R&D section of a company, they will provide a boost to the cooperation among different departments.

- Promote courses and technical careers able to provide expertise in industrial materials modelling and to increase the awareness of the potential in terms of industrial innovation and career opportunities.

5 About EMMC and this Roadmap

For Europe, the EMMC – the European Materials Modelling Council – proposes actions to underpin and enable the industrial implementation and exploitation of modelling as well as digitalisation of materials. Both are considered crucial to facilitating the digital transformation of industry, enhancing industrial competitiveness and supporting the European Green Deal.

The EMMC Roadmap serves multiple stakeholders and purposes, hence the needs of a broad and large community of stakeholders interested and active in materials modelling and digitalisation are identified and discussed. In particular, the Roadmap addresses the State of the Art, defines the challenges ahead, and provides recommendation to achieve the formulated vision. The EMMC Roadmap can hence serve as a guideline for the EC and other relevant bodies of Europe-wide interest to advance and support the recommendations in Horizon Europe calls.

The EMMC Roadmap is based on extensive consultations across the broad spectrum of European stakeholders conducted by the EMMC in the past 6 years. Following the implemented actions of Horizon 2020, continued progress should be made in the Horizon Europe Work Programme 2021-2027. In particular, the EMMC Roadmap recommends continued and further advances for materials modelling and digitalisation and sets criteria to enable a successful transfer and implementation to industry of the overall knowledge, experiences and tools accumulated during the last 5 years. These will foster continuous improvement towards higher levels of maturity in the industrial use of materials modelling and digitalisation leading to a more agile European industry, able to respond to the complex and fast-changing 21st century challenges.

5.1 Disclaimer to the approach

The EMMC Roadmap recognises the importance of making advances in materials modelling and digitalisation to support the competitiveness of European industry. It strives to identify shortcomings and barriers in current approaches and proposes actions to address them based on a rich input and many discussions between the various stakeholder communities. The EMMC has organised and facilitated many of these interactions with and amongst stakeholders who are broadly identified as: materials modellers and data scientists, translators, software owners and manufacturers. However, the EMMC cannot be held responsible or liable in any form for statements made by stakeholders, or potential socio-economic consequences of implementation and use of any of the Roadmap recommendation. All recommendations are based on stakeholder feedback and are presented in good faith. They do however represent the EMMC position of the best possible approach for ensuring environmental, economic or societal impact of materials modelling and digitalisation of materials sciences in industry.

5.2 EMMC- European Materials Modelling Council

In 2019, EMMC represented about 950 members with an interest in materials modelling and digitalisation of materials sciences. EMMC promotes the application of materials modelling to support the European Industrial Competitiveness. The integration of materials modelling and digitalisation is considered future critical for more agile and sustainable product developments and use throughout the entire materials life cycle. It is aligned with the drive towards a digital society that assists in developing a circular economy for addressing urgent societal needs.

EMMC has the goal to network existing and future activities happening in the field of materials modelling. The aim of the Council is to establish current and forward-looking complementary activities necessary to bring the field of materials modelling and digitalisation closer to the needs of industry (both small and large enterprises) in Europe.

In February 2014, 75 experts attended an EC Materials Modelling Policy meeting held at Covent Garden, Brussels. The views were captured in a Report "Materials Modelling: Where do we want to go" published on the LEIT website[10]. The EMMC was created with volunteers who started various working groups (WG) on materials modelling topics of general interest. Discussion notes were elaborated and an initial listing of 600 potential interested people and stakeholders was created and consulted to submit their interests and views. Subsequently and since then, the substantial comments and suggestions received have been captured into the Roadmap 2015. The extension of this Roadmap represented the Roadmap 2016[g], where more systematic inputs were collected by a dedicated online survey, which was sent to more than 1500 stakeholders.

In 2016, EMMC was awarded a Horizon2020 grant for a Coordination and Support Action (CSA). EMMC activities were supported by the activities of EMMC-CSA (see https://emmc.info) from 1 Sept 2016 to 31 August 2019.

In 2017, several EMMC workshops and expert meetings were organised (e.g. EMMC International Workshop 2017[h], EC/EMMC Translation Workshop[i], EMMC Workshop on Interoperability of Materials Modelling[j], EMMC Workshop on Model Quality, Gaps & Accuracy[k], EMMC Business Decision Support System Expert Meeting[l]) with the goal to collect the opinion on different relevant topics for and from a number of stakeholders. The digested reports contributed to the Roadmap 2018, while the consolidated insights gathered over the last 6 years are culminated in the present EMMC Roadmap.

Due to its wide-ranging membership and stakeholder involvement, the views expressed by the EMMC are generally endorsed by a significant number of stakeholders representing the views of a large and open materials modelling and digitalisation community.

The vision of EMMC is to achieve a full material modelling integration and digitalisation of materials sciences in European manufacturing industry, thereby enhancing European industrial competitiveness

---

[g] https://emmc.info/emmc-roadmap-2016/
[h] https://emmc.info/the-first-emmc-international-workshop-2017/
[i] https://emmc.info/events/translation-workshop/
[j] https://emmc.info/events/interoperability-in-materials-modelling-intop2017/
[k] https://emmc.info/emmc-materials-modelling-workshop/
[l] https://emmc.info/events/emmc-csa-bdss-experts-meeting/

The mission of EMMC is to support activities furthering all aspects of materials modelling and materials digitalisation, from strengthening their foundation, to their transfer to industrial use and industrial impact. In a long-term perspective, the improved use and deeper integration of materials modelling and digitalisation throughout the entire materials life cycle will enable a more agile and sustainable development of improved materials and processes.

In order to ensure sustainability of EMMC activities, a not-for-profit association, EMMC ASBL, was registered in July 2019 in Brussels. EMMC ASBL objectives, as stated in its statutes include:

- Improve interaction and collaboration between all stakeholders involved in different types of modelling and digitalisation of materials, including processes and manufacturing. The main stakeholders are modellers, data science experts, software owners, translators and manufacturers.
- Identify the main obstacles to the increased use of modelling and digitalisation of materials in European industry and develop strategies to overcome them.
- Facilitate the integrated modelling and digitalisation of materials on a solid and coherent basis.
- Coordinate and support actors and mechanisms for the rapid transfer of modelling and digitalisation of materials, as well as academic innovation, to end users and potential beneficiaries in industry.
- Support the sustainability of modelling and digitalisation of materials in Europe.
- Increase awareness and adoption of materials modelling and digitalisation in industry, especially SMEs.
- Support the software industry for materials modelling in Europe.

EMMC ASBL is open to membership by individuals as well as European organisations with an interest in modelling and/or digitalisation of materials, processes and manufacturing.

5.3 Stakeholders

The EMMC Roadmap is aimed at assisting multiple stakeholders to accomplish the EMMC vision by realising its mission. Five broad groups of stakeholders can be identified in the diverse and rich ecosystem that develops and utilises models to accomplish more efficient and effective innovation of chemicals and materials and their integration into new products.

- Modellers: all individuals or organisations that develop and use models capturing materials science knowledge in order to describe, simulate and explore challenges related to the design, development, processing and manufacturing of materials.

- Materials Data Scientists: Experts who perform method development and application of data analysis to solve materials science problems in close synergy with other modelling stakeholders.

- Software Owners: Individuals, groups or organisations that develop and provide digital tools and services. It includes academic developers of materials modelling codes and commercial software and services suppliers.

- Translators: Experts that connect manufacturer challenges with potential solutions using materials models and digitised materials sciences knowledge.

- Manufacturers: Commercial (for gain) organisations that design, develop and produce materials and products based on materials knowledge. It includes a wide range of industrial sectors, such as chemicals, electronics, automotive, aerospace, energy, consumer packaged goods and pharmaceutical materials and manufacturing.

5.4 Vision

The vision of the EMMC is to achieve a full materials modelling integration and digitalisation of materials sciences in European manufacturing industry, thereby enhancing European industrial competitiveness.

European Manufacturing organisations have evolved to ‘intelligent enterprises’ able to co-create and co-innovate with its customers and partners in an agile manner. A solid digital materials foundation and a range of materials modelling assets and capabilities that can be readily deployed enable a ‘model first’ approach. In this vision of “Materials and Manufacturing 4.0”, modelling is at the heart of decision making as materials models are fully integrated into the industrial workflows. Organisations generally achieve a high level (managed or optimised) of maturity across its modelling tools, data, workflows and people competences.

Europe has a strong, well educated, diverse, and skilled workforce of academic software owners and developers, modellers, materials data scientists and experts trained in modelling as well as business development. In academia and industry, they support ongoing and future advancements of models and software, translation of industrial challenges into modelling solutions, materials knowledge digitalisation, industrial product development and integration of materials modelling to create the intelligent enterprise.

European software and services organisations are thriving and world leading. The leadership is based on world renowned academic developments in materials science and digitalisation that naturally flow into industry for use in an agile manner via integrated and flexible platforms, cloud-based solutions and digital marketplaces.

6 Acknowledgements

Much of the road-mapping effort has been supported by the EMMC-CSA project which has received funding from the European Union‘s Horizon 2020 research and innovation programme under Grant Agreement No. 723867.

The number of contributors to the EMMC Roadmap is too long to be listed here, but particular thanks go to the partners of the EMMC-CSA project: TU Wien (Nadja Adamovic), Fraunhofer IWM (Adham Hashibon), Goldbeck Consulting (Gerhard Goldbeck, Alex Simperler), Politecnico di Torino (Pietro Asinari, Luca Bergamasco), Uppsala University (Kersti Hermansson), Dow Benelux (Tom Verbrugge), EPFL (Nicola Marzari, Martin Uhrin), DPI (Denka Hristova-Bogaerds), ACCESS (Georg J. Schmitz), Materials Design (Erich Wimmer, Volker Eyert), Synopsys QuantumWise (Kurt Stokbro, Umberto Martinez), Granta Design (Donna Dykeman, David Cebon, Davide Di Stefano), University of York (Roy Chantrell), University of Bologna (Emanuele Ghedini), to Rudy Koopmans (Koopmans Consulting) and the EMMC Industrial Advisory Board members as well as to the EC Project Officer for the EMMC-CSA project, Anne de Baas.

7 References

---

[1] 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.

[2] Review of Materials Modelling: "What makes a material function? Let me compute the ways…", Anne F. de Baas (ed), 6th Version (2017), DOI: 10.2777/417118

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

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

[5] https://zenodo.org/record/3552260

[6] White paper for standards of modelling software development, https://zenodo.org/record/1240212

[7] Business Models and Sustainability for Materials Modelling Software, https://zenodo.org/record/2541723

[8] The Economic Impact of Materials Modelling, https://zenodo.org/record/44780

[9] Strategies for industry to engage in materials modelling, https://zenodo.org/record/3564455

[10] “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