3rd EMMC International Workshop 2021

Report - Short version

EMMC ASBL

The European Materials Modelling Council

Responsible for content:

EMMC ASBL

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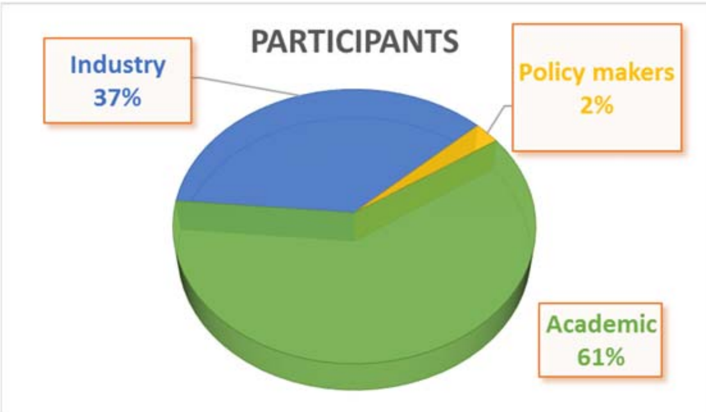
Introduction

The EMMC International Workshop has become known as a leading cross-cutting event where experts from materials, manufacturing and software industries, academia as well as policy and funding stakeholders get together to discuss topics of strategic importance in materials modelling and digitalisation. It is unique in bringing together all types of modelling as well as data science relevant to industrial impact. The format of Discussion Sessions, with prepared Discussion Notes and Impulse Talks by leading experts lends itself to open yet focussed discussion about gaps and potential actions to move the field forward.

Following previous workshops in Vienna in 2017 and 2019, the 3rd EMMC International Workshop 2021 (EMMC 2021) took place online from 2nd-4th March 2021.

There were 250 registered participants, mostly from all over Europe as well Israel, Algeria, USA, Canada and Japan. There was again a very significant participation from industry as shown below.



The programme of the event included seven plenary presentations, twelve Discussion Sessions as well as Open Contribution session with online poster and meeting opportunities.

EMMC would like to thank the fantastic community effort in organising and running the event and all speakers and participants for their valuable contributions.

This report was made possible by contributions from Nadja Adamovic (EMMC and TU Wien, A), Maria Alfredsson (University of Kent, UK) Silvia Chiacchiera (STFC, UK), Malgorzata Celuch (QWED, PL), Davide Di Stefano (Ansys, UK), Donna Dykeman (Ansys, UK), Volker Eyert (Materials Design, F), Gerhard Goldbeck (EMMC and Goldbeck Consulting Ltd, UK), Giuseppe Fisicaro (CNR, I), Jesper Friis (SINTEF, NO), Adham Hashibon (Materially, D), Kersti Hermansson (Uppsala University, Sweden), Denka Hristova-Bogaerds (DPI, NL), Esther Hurtós (EURECAT, E), Glenn Jones (Johnson Matthey, UK), Peter Klein (Fraunhofer ITWM,D), Natalia Konchakova (Hereon, D), Gabriele Mogni (Goldbeck Consulting Ltd, UK), Nawfal Al-Zubaidi R-Smith (JKU Linz, A), Georg J. Schmitz (ACCESS, DE), Michael Seaton (STFC, UK), Alexandra Simperler (Simperler Consulting, UK), Ilian Todorov (STFC, UK)

Note: The Discussion points sections pose questions of interest to the community and how they were answered by the contributors to the respective Session.

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Model Development

This Focus Area represents everything that has to do with the **capabilities** and **quality** of materials models and modelling workflows. Development and validation of models and workflows belong here as do their application to challenging problems of industrial relevance in a range of application sectors.

Physics-based models and modelling, and data-driven AI/ML techniques to support them, have a firm place in this focus area. The models and methods involved are...

- Models from the electronic and atomistic scales up to the continuum world
- Coupling & linking, i.e., multiscale modelling, hierarchical techniques
- Modelling approaches to describe-understand-predict materials properties and processes
- Modelling to interpret experimental properties
- Machine Learning to develop interatomic potential and atomistic models
- ... and more.

This Focus Area is the home of individuals and organisations – from industry and academia –interested in promoting these or similar topics.

Electronic, Atomistic and Multiscale Modelling: Why should Industry care?

Objectives

The objective of this session is to gather information on

- how European industry perceives the role of atomistic and electronic scale modelling for future development
- what the most urgent barriers are to overcome in industry and academia to strengthen the role of modelling in general
- how to best achieve synergies between physics-based and data-driven modelling (collect successful and not so successful examples).

Introduction

Numerical simulation in industry today is to a large extent dominated by continuum Structural mechanics and Computational Fluid Dynamics models. They form part of a Computer Aided Engineering design process that started more than 50 years ago and is now regarded as a mature discipline. It is widely adopted in industry and served by a number of multi-billion Euro software companies.

So is there room for, and a need for, materials modelling at the electronic and atomistic levels for industrial problems?

The answer should be yes, as there is a need from industry and society for materials and molecules with tailored electronic, atomistic and nano-scale functionalities. Even the engineering of these materials often relies on controlled electronic and atomic-scale processes. All this is an opportunity for materials modelling, but it is also a challenge to link the microscopic scales to the real world. Capable and reliable models and workflows (physics-based and/or data-driven) will be needed.

The session as a whole is titled Modelling Advances, and the subtheme is the question above: "*Is there room for ...*?". Our three impulse speakers, and the ensuing discussion, will highlight a range of aspects of how electronic and atomistic modelling can make itself useful, and how weaknesses and scepticisms can be tacked.

Discussion points and questions

- **Will the role of electronic and atomistic modelling in industry become stronger or weaker in the future? Will it perhaps be an expertise exercised by academia only, possibly with industrial funding?**

Future will observe an increasing role of electronic and atomistic modelling. Modelling at atomistic levels, employing both at *ab initio* as well as other computationally less expensive approaches, will support enormously almost all fields of material science. Material design and material discovery, properties or process simulations will support experimental studies to foster and speed up all relevant production steps at the industrial level. The Horizon Europe program together with its global target objective cannot forbear of making advantage of current electronic and atomistic modelling approaches. Production chains into micro and nanoelectronics, photovoltaic, electrochemical cells and batteries, quantum computing, pharmaceuticals, agriculture, health as well as informatics are examples of areas that can all benefit from modelling and calculations at an atomistic level.

Academia should pursue fundamental research in terms of modelling and theory, developing/testing and validating the instruments that will serve industry in their innovative applications. An example is the development and maintenance of Neural Network Potentials, databases and workflows like the AiiDA platform, which need large resources and time available at the academic side. Then Industry can take advantage of such state-of-the-art modelling tools. It is of the outmost importance that a continuous dialogue between all stakeholders both on the academic and industrial side occurs, maybe in the form of collaborative research projects, to answer relevant questions in the correct framework.

- **Are there really good examples of how atomistic and electronic-scale modelling can be used to reduce development costs? Or is the value of insight enough?**

There are many good examples of how atomistic and electronic-scale modelling can be used to reduce the development cost. For example, large screening of databases storing materials properties can enable the design and discovery of materials to be synthetized. The same hold for structure predictions simulations. In his plenary, Prof. Nicola Marzari showed a database search of all layered materials with the discovery of new two-dimensional compounds. A similar investigation cannot be possible with a solely an experimental approach.

Development cost can be strongly reduced by means of process simulations. For example, Kinetic Monte Carlo simulations can aid with the optimisation of the process conditions regarding the growth of epitaxial layers or patterned substrates and lead to a large reduction of the development costs.

- **Where will we be 5 years from now? 10 years from now?**
  - **concerning the role of electronic & atomistic-scale modelling**
  - **concerning the capabilities (and use of) of multiscale modelling**
  - **the trust in modelling**
  - **the esteem for physics/science-based modelling**

Electronic and atomistic modelling have already a role in the research and development department as well as in the production area of many industrial players, e.g., various chemical, pharmaceutical, biological, micro and nanoelectronics companies. However, new computational techniques, like machine learning for interatomic potentials or material properties models, material design from databases, robust and reliable library like OpenKIM[1] or simulation platforms like AiiDA can boost target technologies.

Multiscale modelling is already on the materials modelling market, where first-principles properties can be used as input parameter for simulations, which allows time and space scales typically needed for industrial problems and processes.

[1] https://openkim.org/

We are in the middle of a paradigm change, where traditional academic codes, freely available for non-profit research without a graphical user interface, now are evolving into user-friendly software, where codes are well enriched with regression tests, tutorials and documentation. With the increase in computing power and, therefore, the number of jobs, or simulations, that can be run, academics find themselves developing code to run their simulation software and collate their data. In doing so, they are also evolving their code towards more robust software which can be easily integrate in multiscale problems or simulation workflows.

The increasing benefits from materials modelling will increase the esteem on the whole computational activity.

- **Will future companies have the need to set up an AI department for production development?**

Organisations should not underestimate emerging digital technology. Investments in AI departments for production development will be rewarded. Data analysis, process and manufacturing modelling can strongly support the production area, speed up the whole chain and reducing efforts as well as material/energy lost. Furthermore, electronic and atomic scale simulations can allow the monitoring, and by consequence its understanding, of the system/process evolution at scales which are totally inaccessible at the laboratory level. For example, evolution of material components at atomic level during nanosecond laser annealing or interactions of a molecules or photons at the catalytic regions of target materials.

Final remarks

- Multi-model and multiscale approaches, using accurate interatomic potentials, databases, as well as machine learning techniques has been enabling the modelling of large systems and speeding up the exploration of target materials while retaining and improving accuracy.
- There have been big advances in combining physics and ML models and these will be used very widely in industry in future.
- Modellers in industry need a broad range of skills from technical to people oriented.
- Academic codes, freely available for non-profit research without a graphical user interface, are evolving into user-friendly, robust software.

From Modelling to Experimental Characterisation for Energy Materials

Objectives

The main objective of this session is to encourage new efforts of the EMMC community towards the modelling of energy materials. Specific collaborations are sought in:

- multi-scale multi-physics modelling of energy materials,
- data-based modelling of energy storage materials and devices,
- Open Platform modelling tools and examples for energy materials, for education purposes,
- Linking & Coupling Computational Chemistry to Electromagnetics (proposed Task Group),
- linking MODAs and modelling results to CHADAs and characterisation results.

Introduction

The session aims to correlate computer modelling and experimental characterisation, in application to the increasingly important area of energy materials. Two thematic sub-areas are first addressed: solar cells and batteries, and applications of both physics-based and data-based modelling approaches are considered. Discussion will be directed so as to identify key research problems relevant to the modelling of solar cells, taking into account characterisation data for organic semiconductor materials. Further, industrial problems relevant to the modelling of Li-ion batteries will be discussed, as exemplified by the modelling-based detection of material defects in graphene anodes or separators.

Following the impulse talks, broader discussions and collaborations within the EMMC are envisaged to follow. Expertise in multi-scale multi-physics modelling of energy materials is specifically solicited as well as joint efforts for the development of Open Platform tools and examples, for teaching and public communications on the subject. Collaborations are also sought with the sister society, EMCC, facilitating a MODA of each modelling example to be linked to its corresponding CHADA and characterisation results.

Discussion points and questions

- **In what respects are energy materials *different*? To what extent the existing EMMC competencies are applicable?**

Energy materials are generally complex, and the material parameters are various with strong coupling in between them. Thus, multi-physics modelling is required, and modelling should be combined with user expertise and proper characterization methods to properly model the material.

- **Does characterisation data sufficiently substitute for the missing knowledge of the physics of energy materials? Can data-based modelling foster further developments in the physics?**

Several characterization data and methods for energy materials are available or under development. However, the characterization itself is not sufficient if not supported by modelling techniques. Modelling can be applied for example to improve the performance of the characterization methods or obtain further insight into the material and the physical and chemical processes. Data-based modelling can help to better interpret the electrochemical process that are probed using some characterization methods (e.g., EIS), and the models can be combined with some other methods in order to predict states of the battery (SoC, SoH).

- **Is it feasible to perform multi-physics modelling, coupling computational chemistry to electromagnetics?**

In some Multiphysics modelling environments different Multiphysics have been coupled and good results are achieved, while properly coupling the correct elements in the different physics and defining suitable boundary conditions. Examples in this Session have been presented in Comsol (FEM) and QuickWave (FDTD). In organic electronics such multi-physics modelling is a challenging bridge that is still to be built.

- **Are our modelling efforts compatible with the needs of industry, in the fields of energy storage and harvesting?**

Modelling has been or is under development to be applied in industrial environments along with characterization method hardware. An example was presented by Keysight, where adapting data-based modelling to characterization methods to obtain specific parameter information from LIBs and classify cells or provide knowledge on their performance and safety. Other examples are the modelling of characterization methods for inline quality assessment at different stages of battery production lines. Similarly, the use of EIS for industry was recently demonstrated in the field of organic photovoltaics. The method, protocol and associated model was successfully implemented on an industrial pilot line. The method was shown useful for material screening prior to deciding which OPV materials and architectures are worth for industrial manufacturing. This experience however demonstrated that industrial implementation of modelling is enhanced when the model is simple and understandable, hence described by a simple characterization protocol, or, if complex, ease of use for the industrial operator.

- **Can we increase popularity Open Modelling platforms? Will they compete with commercial software?**

Interest in Open Modelling platforms is increasing, especially for academic purposes or R&D groups. The possibly to use the software and model examples openly and freely is important to support and develop characterization methods and the sciences behind them.

- **Is it feasible to try and link every MODA to a corresponding CHADA? Will the twinning of modelling and characterization data increase the trust in both?**

Linking MODA to a corresponding CHADA should be feasible, for example a CHADA already contains a workflow to link several characterization methods by showing the link or correlation between these methods. A similar process can be followed to link CHADA and MODA. The link between both is important as this can improve the results of the characterization method and simplify the understanding of it. Additionally, connecting MODA/CHADA and several ones together is of high interest of the industry due to the necessity of several characterization and modelling at different stages such as for example battery production lines.

- **How to increase public awareness of modelling for energy storage? Could modelling act as a saving mechanism to foster development of energy storage?**

A key element for the development of energy storage is modelling, data-based or physics based. Modelling can support in improving the design, geometry or performance of energy storage or their characterization methods. As well as applied to characterize and estimate performance and state of energy storage applications.

Final remarks

- Modelling is essential for proper energy materials characterization and development. As well as its important for performance and defect analysis of batteries.
- Multiphysics coupling is important for energy material modelling due to their complexity and influence of several coupled parameter
- Connecting MODA to their relevant CHADA can be very valuable and improve the characterization process.
- MODA & CHADA is an important combination, e.g., for interoperability, or industrial application several MODA or CHADA are required and ought to be combined and this is then more applicable to industry in a broader sense.
- There is a lack of common interface coupling from different available modelling tools. For example, some commercial software is coupling physics in “some way” and we need to understand how the physics works by coupling and not only the mathematics behind it, thus it is important that some “common” is set.

Interoperability

This Focus Area represents everything that has to do with interoperability, which is the ability of two or more systems to exchange information through a common representational system to perform complex tasks that cannot be done by each single system alone.

The aim is to reach the highest level of generalisation leading to a range of benefits including that no privileged one-to-one connection between systems is required nor desired and to aim for linear scaling of interoperability operations as more systems are added, rather than power scaling for one-to-one compatible systems. An agreement on a common representational system also facilitates standardisation of computational interfaces as well as standardisation of documentation, based on underpinning metadata, taxonomies and ontologies.

Ontologies for Interoperability

Objectives

The scope of this session is to bring key stakeholders together to foster wider collaborations and ensure alignment developments in order to mitigate the risk independent actions will threaten the overall interoperability goal. In addition to illustrate examples of application ontologies, impulse talks will elaborate on how ontology boost interoperability, including how to get from individual actions to a coherent and harmonised system and how to make ontologies interoperable.

Introduction

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. Recently in the material science domain, various international actions identified ontologies and related information technologies as critical tools for interoperability. Semantic approaches to interoperability arose out of the need to integrate databases having their own data vocabulary, however these have gain attention as ways to facilitate interoperability between heterogeneous materials modelling software in complex workflows.

Discussion points and questions

- **How can ontology help interoperability?**

Having interoperable/integrated data is relevant to make data not only FAIR but also AIR (=AI ready). Application Ontologies do already find their way into industry and their possible uses are: unify, build standards, integrate data, and make knowledge explicit. A caveat may be that ontologies contain our view of the world, so they entail subtle choices. Hence, one has to be aware when adopting one. A few examples of applications were presented: in manufacturing, in chemistry (semantic annotation of journals) and for simulation data. Further examples of knowledge sources (e.g., IUPAC colour books) evidence that experts are discussing still convergence.

Specific examples are:

1. NOMAD lab and its metadata schema for atomistic simulations; they enable data query and analytics
2. Royal Society of Chemistry projects lead to two open-source ontologies for chemistry CHMO and RXNO. CHMO - Chemical Methods Ontology (sample preparation etc.) and RXNO - Reaction Ontology (to classify reactions)

3. Ontological modelling of manufacturing resources (Applied Ontology, vol. 16, no. 1, pp. 87-109, 2021 by E. Sanfilippo et al.)

Final remarks

Harmonisation of foundational ontologies and generating a modular, amendable and freely configurable set of (domain-) ontologies seems to be an important challenge. One prerequisite for such a configurable system of ontologies seems to be the restriction to a well elaborated and sound set of relations between classes, which should be common to all ontology modules.

The topics

1. How to get from individual actions to a coherent system?

and

2. How to make ontologies interoperable/harmonise between them?

should become subject of future EMMC task groups.

Interoperability in Practice

Objectives

The scope of this session is to bring key stakeholders together to increase awareness of and harmonisation between ongoing interoperability initiatives as well as to foster wider collaborations and support aligned development. Focus will be given to tools to work with ontologies and challenges, requirements, and lesson learned from interoperability success stories.

Introduction

Material science is evolving from tightly and syntactic connected modelling workflows into more flexible workflows consisting of loosely connected and replaceable modelling software and databases. To exchange data with unambiguous, shared meaning between such loosely couples modelling software that may have been developed independently of each other by groups from different disciplines using different terminology demands an increasingly more explicit and machine-interpretable semantics. Ontologies in the form of logical domain theories and their knowledge bases offer rich representations of machine-interpretable semantics for systems and databases in the loosely coupled world, thus ensuring greater semantic interoperability and integration.

Discussion points and questions

- **What are the benefits of semantic interoperability over syntactic interoperability?**

According to healthcare specialists, semantic interoperability enables "… *exchange, interpretation, and use of data across disparate systems.*"[2]

- **What is semantic interoperability? Is it often confused with syntactic interoperability with terminology extracted from an ontology?**

"*In general terms, there are two types of interoperability: syntactic and semantic. Sematic interoperability is more desirable than syntactic interoperability. With semantic interoperability, the data is not only exchanged between two or more systems but also understood by each system. Syntactic interoperability allows two or*

[2] https://www.carecloud.com/continuum/what-is-interoperability/

more systems to communicate and exchange data, however, the interface and programming languages are different."[3]

- **How can ontologies help interoperability?**

This should be tackled by an EMMC focus group – the "killer application" is still missing. There is an urgent need to collect contemporary use cases.

- **Identify low-hanging-fruits of interoperability – use cases and practical applications?**

This should be tackled by an EMMC focus group – the "killer application" is still missing. There is an urgent need to collect contemporary use cases.

- **How to reap the benefits of interoperability with respect to cost/time/expertise/reusability/ resilience/…?**

Should be tackled by use cases.

- **How to increase awareness of importance of interoperability – ensuring that people take interoperability into account in early enough in the design phase…?**

A task group should be formed that collects best practices.

- **How to design for and increase interoperability?**

A task group should be formed that collects best practices.

Final remarks

An intense discussion about "efforts" will be necessary. The efforts are to maintain ontologies, make them secure and to find financial means to do this. Many "old ontologies" are lost – thus, repositories are needed. Building a community is key, so EMMC should interact with the OntoCommons CSA.

Digitalisation

This Focus Area represents digitalisation which refers to the process of making use of digitised information (i.e., data in a digital form) to formulate and to create new knowledge enabling the extraction of insight out of such digital data. The overarching goal of this Focus Area is to create a vibrant digital materials development eco-system in Europe that encompasses all the above activities and links them together to Open Translation Environments, Innovation Test Beds, Open Characterisation Hubs and Environments, Manufacturing Marketplaces and Open Innovation Platforms and Findable, Accessible, Interoperable, Reusable (FAIR) Materials Data Repositories.

Digital Marketplaces

Objectives

The main objective of the session is to foster information exchange and open discussions between various platforms and the EMMC facilitating an enhanced coordination towards sustainable progress of digital

[3] https://www.electrosoft-inc.com/resources/syntactic-and-semantic-interoperability

marketplaces. Key aspect is the identification of the main challenges and progress inducing actions needed. Specifically, the objectives are:

- Bring together and network existing collaborative platform owners, developers, and users.
- Identify key business aspects and long-term sustainability challenges and prospects.
- Public-private partnerships versus commercial, the interplay and possible roles of public and commercial platforms.
- Multisided versus single sided platforms, pros and cons for the community.
- IP and user management/privacy needs, current and future aspects.
- Can the EMMC serve as a public marketplace? What is its scope? How to integrate and lead the way for commercial augmented solutions?

Introduction

EMMC Digital Marketplaces are multisided collaborative platforms, typically utilising cloud technologies to facilitate the sharing, collaboration, curation, discovery and creation of new insight and knowledge. They typically include integration of several components that can range from translation, digitalisation of research data (covered by a separate session) to education and training and materials modelling applications, requiring thus efficient exchange powered by interoperability between all components. This session is focused on discussing the various interplays between these components, and between various available and emerging public and commercial marketplace platforms.

Discussion points and questions

- **How to manage data provenance over the entire landscape of platforms and applications. Is this possible/wanted/desired/needed (and by whom)?**

Each provider is managing the data provenance in their eco system. There is some appetite to look into widening the ecosystem – only then it will be necessary to look into augmenting data provenance.

- **Bridging the gap between FAIR requirements and applications: how can information/knowledge be findable? How can it be accessible, what level of interoperability is needed? What are the conditions for reusability?**

Data, of course, is a fundamental prerequisite, but it's not just a matter of making data searchable and accessible, it's a matter of extracting value out of it, and that can only be done by very well-thought and fine-tuned services. Thus, the service provision will dictate what the FAIR requirements will have to be.

Also, some marketplaces are repositories and others provide the data tools – this requires a high level of interoperability.

- **Can or should the community of digital platform providers agree on minimal FAIR requirements with respect to actual features? Will this benefit all platforms?**

All digital platform providers have FAIR principles in place. However, the FAIR data principles are very simplistic and insufficient, since everyone can interpret the different letters in different ways. Having the standards set for this is needed. In the long run, all these platforms will definitely want to be able to exchange information in a smart way.

- **IP and privacy, how to cater for more industry needs for confidentiality? Technological versus legal aspects. Do we need a global agreement with minimal requirements?**

So far, each provider has measures in place to cater for their industrial customers. However, we need to establish connectors between market places first and develop “global agreements” in tandem to that.

- **How to create more synergy between existing players (domain providers)?**

Especially the DOME project is aiming to develop a connector, that allows every platform to share data, including the conditions on how to share data, how to monetise it, whether it's a virtual common currency or not (e.g., Bitcoin). VIMMP, MatMatch, MaterialsZone, Materially, DOME and others would then be able to share some kind of data as a common ecosystem, and as a common critical mass. Ultimately, the platform owners need to ask these questions to the users eventually. There is a lot of discussions and decisions to be made on the conditions of the sharing of data with the users and with other platforms, to make sure that everybody benefits. Users have the interest of data circulating as much as possible. Some clear restrictions would have to be put in place, but the raw data could certainly be available to everybody.

- **Future needs from users and providers.**

There is a need for a joint eco system and connectors between platforms, that would greatly increase the value of the data contained in them. It might be a good suggestion to have a specific task group on interfacing data between the platforms, that will discuss the various conditions for this to be possible (legal aspects, monetising and other aspects). A poll conducted during the session showed that 91% were in agreement of sharing data across such an ecosystem of platforms. Another poll revealed that 62% of the audience thought that the data itself is the product, but a non-negligible 36% sees the services as the product.

All marketplaces require a critical mass of data to actually be productive, profitable and sustainable. This raised the idea to concentrate on creating an overarching ecosystem as the way forward and establish a connector so that the user in the end gets the added value through a seamless interface.

Final remarks

- Having interoperability of tools and the different ways data ends up being represented semantically is a crucial ingredient that EU and the community in general needs to tackle.
- There is a need therefore to have a more stringent, clear, and specific definition, and agreement on what FAIR actually means and implies on a practical level. This is lacking, hence currently this is merely representing a general vague concept that is open for much interpretation, explaining the high degree of fragmentation in the domain.
- There is a need to clear legal frameworks that govern IP and access rights, without these, there is too much scatter in the way each platform treats this issue and hence no trust from industry can be built.
- There is a need to design and provide easy to use API and interface/connector aggregators, these enable any system or marketplace or data warehouse to connect to another, however, the connectors require much maintenance, and while there is a societal common benefit to all from such connectors, their business case may be undefined. Hence, there is a need for supporting such connectors based on public funding.
- There is a need therefore to have a more stringent, clear, and specific definition, and agreement on what FAIR actually means and implies on a practical level. This is lacking, hence currently this is merely representing a general vague concept that is open for much interpretation, explaining the high degree of fragmentation in the domain.
- Having interoperability of tools and the different ways data ends up being represented semantically is a crucial ingredient that EU and the community in general needs to tackle.

Digitalisation of Research Data

Objectives

The immediate objective consists in diversifying the activities of the EMMC in digitalization. For this purpose, a dedicated exchange is needed that addresses major fields of activity in digitalization for materials modelling, including in particular 1) digitalization of literature data and 2) research data infrastructures. It will be discussed whether task groups along these lines should be established within the EMMC ASBL organization.

Introduction

This session addresses ongoing activities and plans concerning

- the development of research data infrastructures,
- digitalization of journal data,

providing an opportunity for coordinating between initiatives and planning joint work. It will be discussed what metadata standards are in use (e.g., MODA, metadata schemas, and ontologies), and how alignment and mediation between infrastructures and journal-publication based knowledge graphs can be supported. The landscape of European-funded projects, including within EOSC, will be evaluated and situated in a global context, in particular as regards the Horizon Europe programme.

Discussion points and questions

- **What metadata standards and agreements on good/best practices in dealing with materials modelling data exist from external (not EMMC-related) initiatives? What steps need to be taken to align them with EMMC-associated efforts?**

There are a number of actions and most, with the exception of the EOSC, are not based on ontology but rather on syntactic data formats like EnzymeML and others. The Material Digital project is fostering the creation of ontologies in isolation of the EMMC, which may lead to further fragmentation. The EOSC projects contribute actions towards a federated semantic artifacts data space which may help remedy this fragmentation.

- **How can we best support the digitalization of all data from papers published in journals and other (non-paper) publications of research data in the field of materials modelling, while advancing the uptake of FAIR principles of research data management?**

There is a need to integrate FAIRness of data right into the process of the data creation, i.e., there is a need to shift the way experiments and simulations are executed in order to allow to capture data and metadata in real time. As for papers, this has not been touched directly; however, we can assume that when such a process is put into practice then it will be straightforward to augment papers with fair data more readily.

- **What does the landscape of emerging and pre-existing research data infrastructures look like, concerning materials modelling? How can we support these diverse platforms at becoming interoperable – and the underlying standards at becoming aligned – with each other and with platforms and infrastructures developed from EMMC-related projects?**

It seems highly fragmented but there are many overlapping actions; the role of the EMMC and related projects like OntoCommoms should act more agile to bring all actions inline. The idea of a federated semantic artifact space is good and should be perused.

- **In view of this, what do we as a community want to recommend for Horizon Europe proposals and projects to prioritize in their work programmes concerning digitalization?**

Actions to align semantic artifacts from various domains under the same umbrella, include many domains and actions from e.g., EOSC and other national actions. There is also a need for tools enabling the development of standards and common data formats.

Final remarks

There is a clear misconception regarding what the role of metadata, ontology and FAIR is. More work to clarify this is needed and this could be reached by establishing task groups with the EMMC.

There are numerous ongoing actions from all domains, and EOSC is laying the ground for guidelines that the materials community in general and EMMC should tap into. Metadata seems to be a good start for building ontologies, but synchronising work is needed. There is a severe lack of actual implementation which is understandable as the community are in the early phases of the specification of guidelines. A major effort is the need to connect ongoing practical ontology-based implementations from the materials domain based on EMMO with those of experiments and processes. This calls for more detailed analysis of the existing ontology actions and how to link them, which is something ongoing also in the H2020 Project OntoCommons. There is a need to understand how the PID concept can fit into the EMMC actions and roadmaps.

Software

The main purpose of this Focus Area is on motivating, facilitating, and promoting the transfer of software for computational materials science into ready-to-use tools for industry, and on providing a forum especially for industrial end users to express their evolving requirements for materials modelling software.

Industrial Requirements to Materials Modelling Software

Objectives

The main objective of this session was to identify the requirements of industrial end users to materials modelling software in order to prepare guidelines for future developments and eventually for the upcoming EMMC roadmap.

Introduction

While materials modelling software is playing an increasingly important role in industrial research the widespread use of these tools is still hampered by a variety of factors. A fundamental issue is posed by the different perspectives of (mostly) academic software developers and industrial end users. Listening to each other and clarifying expectations is thus of key importance for further progress. Addressing the end-user's point of view this session will be concerned with identifying the requirements to materials modelling software. In this context, key aspects include ease of installation, robustness, ease of use, accuracy, complexity, interoperability, performance, training, support, and maintenance. Impulse talks by experts in the field will initiate a discussion about actual and future requirements of industrial end users for materials modelling software.

Discussion points and questions

- **What are the key requirements for adopting materials modelling software in industrial research? Robustness? Usability? Interoperability? Performance? Training, long-term support, and maintenance?**

To adopt a particular material modelling software package, an industrial company needs to be able to obtain (purchase if necessary), install and maintain it in a corporate computing environment, which requires the following properties:

1. Code stability to minimise the number of required bug fixes (links in with robustness)
2. Meticulous documentation of any third-party software
3. Safeguards to ensure commercially sensitive data are protected
4. Ability to work with network security measures
5. Prompt and professional customer support
6. Ability of developers/providers to negotiate administrative hurdles

If in-house or commercial software incorporates open-source code/libraries, licenses for the latter need to be sufficiently liberal (e.g., MIT, BSD) to enable commercial exploitation. (For a company owning its own in-house software is not essential but it can make dealing with internal administration and computing environments significantly easier.)

The software should be able to model materials in the required industrial (technological) context and be able to use (interoperate with) available materials databases and other simulation or analysis tools.

- **Which additional information is needed to improve management's understanding of the benefits of materials modelling?**

What materials modelling can achieve: numerically correct engineering of materials as a direct substitute for real-life experiments, categorically correct exploration of materials to identify candidates for more detailed experiments, conceptually correct evaluation of materials to verify their general behaviour or gain insight into underlying physical principles. Being able to demonstrate that materials modelling is essential to the business, particularly improving on what it currently does, can be persuasive with managers: internal selling of materials modelling techniques to management is frequently necessary.

- **In which ways must materials modelling software be improved to find wider acceptance in industrial contexts? Are there fundamental issues still to be overcome?**

Software usability/accessibility - e.g., enabling non-experts in materials modelling to run simulations - can be key to a particular software package/code gaining industrial acceptance. Being able to link together data from experiments, literature and different simulation methods to compare models at multiple scales and even develop multiscale models of products or processes is a desirable goal for industry: the heterogeneous nature of these data and their different formats are obstacles to automating these kinds of workflows. Generalised platforms that cover multiple approaches to solve both niche and more general problems (built upon available expertise and any unique techniques and/or methodologies) are also highly desirable.

- **How well does training and translation address the information needs of management and decision makers?**

Close communication between software developers and customers (users and their management/decision makers) can be beneficial in translating industrial problems into achievable simulation workflows and the software required to carry those out.

From Materials Science Software to Industrial Tools

Objectives

The main objective of this session is to suggest guidelines to extend the capabilities and applicability of materials modelling software for industrial use. This includes identifying the necessary steps to be taken by (academic) software developers towards professional software development.

Introduction

This session will focus on the journey from academic materials modelling software to robust tools for industrial use, with examples and tips from experts in the field. Overall, it takes 10 to 15 years to move academic software to marketable software. To shorten this, innovation and incubation centres at academic institutions can play a major role. Additionally, academic researchers can benefit from introductory business and market training. It is furthermore recommended that academic developments are initiated using a permissive licensing scheme (BSD or Apache), since that's compatible with commercial tool vendors software downstream the innovation chain. Also, the transfer of academic software to industry should be supported more strongly by the scientific community. The continuity of researchers (ending their PhDs, …) is a challenge for long-term academic R&D work. On the industrial side, software companies should ensure to stay familiar with the state of the art to steer their R&D efforts, avoiding to re-invent the wheel, keeping pace with innovation to match with market needs and focusing on commercialization aspects. Impulse talks by experts in the field will illustrate ways for better transfer of materials science software into industrial tools.

Discussion points and questions

- **What is the optimal way to make academic software developers aware of the key issues need to be addressed in an early stage of software development?**

As an optimal way to make academic software developers aware of key issues from an industrial point of view, it was suggested to enforce and pursue collaborations between academia and industry from the beginning. This boosts the overall process. However, this is a case-by-case situation; the European Commission has the power of funds and could focus on common projects that can help the dialog between all stakeholders.

- **How can commercial software providers support early-career software developers in taking good design decisions?**

This is the major current issue to be address by our materials modelling community. Among others, he noticed that we do not have a career model for the scientists that build computational science and its infrastructure (as opposed to synchrotrons, radio-telescopes, supercomputers, …); we do not have a funding model for the infrastructure of computational science; if we hadn't had the developers of VASP and CASTEP, the field of computational materials science worldwide would be now lagging 10 years behind. Thus, a first step to support early-career software developers his to create such career models.

Furthermore, it is of utmost importance to start communication channels between early-career software developers and commercial software providers at the very beginning of software developments, where code design or licenses schemes have to be fixed. Early-career software developers have to be clear about the licenses that allow future deployments of their codes at commercial level. Right now, the community ask for LGPL compatibility or simply for software that is available. However, licencing is more important than technical capabilities.

- **Which additional information is needed to improve the understanding of academic software developers of the industrial requirements of materials modelling?**

The most effective way to foster the understanding of academic software developers of the industrial requirements is by joint research projects. The reaching of project goals with collaborative daily tasks can provide the optimal environment to growth the awareness from both sides. High technology readiness levels (TRLs) for such projects will ensure the transfer of fundamental research to industrial applications. What may be encouraged is reproducibility, since it is important that research can be replicated. Code should be designed in this way to speed up the transfer.

Final remarks

- There was interest in the audience to look into free and open-source software and to generate a win-win situation for FOSS developers and commercial software providers.
- How can we as EMMC align with national efforts such as the Software Sustainability Institute (https://www.software.ac.uk/) who, according to their webpage, are actively looking into "helping people build better software, and they work with researchers, developers, funders and infrastructure providers to identify key issues and best practice in scientific software".
- Similar to the EMMC Translator, can we align with the UK driven effort of establishing Research Software Engineer, see https://society-rse.org/.
- How can we as EMMC foster access to business education for academic Software Developers? Market research, etc.?
- How can we bring in Professional Software Developers as Mentors and Sponsors into world of Academia?

Impact in Industry

This Focus Area is concerned with all dimensions that play a role in impactful use of materials modelling in industry, in particular People (e.g. Training, Translators), Processes (e.g. Translation, Integration of materials modelling into business workflows), Models (e.g. readiness and management of software, integrated platforms, multi-scale modelling) and Data (e.g. documentation, management, analysis).

New Developments / Views on Translation and Training for Companies

Objectives

Discuss the business model for Translators, their training, operation fields and the need to re-define the Translator role.

Introduction

The Focus Area Impact in Industry has two precursor working groups (WG) of the EMMC, the WG Translation and Training for Companies and the WG Industrial Integration and Economic Impact. While Translation dealt with the transformation of industrial questions to modelling workflows, the Industrial Integration focused on the wide adoption of modelling by the industrial end-users and on the impact of modelling on their business.

One basic idea of the new Focus Area Impact in Industry is to combine these two strands, to build upon the results of the precursors and advice coherent ways for co-creation of innovations by collaborations between industry and modellers, mediated by an advancement of the Translator role.

Discussion points and questions

- **Academics, software companies, internal industry translators and "independent" consultants as Translators: what is the need, the operation field and the business model for each of them?**

1. For all types of translation digital support for agile data analysis and business-related question optimisation are needed.
2. Need of tools for design and analysis of options. Simple optimisation is extremely needed, the complex optimisation could be better!
3. Validation technique, data and partners
4. Simulation is still not fully trusted by many companies. Translators still have to do more in this direction, to increase the trust in modelling. Show cases can help.
5. There is need for a Champion who convinces the management and other layers in the company in modelling.
6. It is important to have a systematic model offering with different ways to approach companies. Engaging all levels also in SMEs can facilitate the adoption of modelling.

- **Is there a need to re-define the role of the Translator?**

No needs to re-define, but the extension of tools to provide effective translation is needed. Moreover, Translators need to be able to build a long-term strategy for a successful partnership with other industrial players and academia.

A working program for Translators could be formulated (based on the talk of Rudy Koopmans):

- Circular, sustainable economy: understand the relation to a complicated and complex eco system.
- Go for a holistic or system kind of thinking; even at the level of company internal functions.
- Materials modelling needs to get integrated towards system thinking. System Models will answer "what-if-questions" at a system level: multi objective decision making necessary.
- More data are not necessarily the answer: we need the right data, related to options in order to take informed decisions. The quality of data is an important point.
- Apply a BDSS: to define what options are possible, getting more quality data is not necessarily enough but need to consider all aspects of the problem and involve experts with various expertise.

Comment from SWO perspective: After the SMEs are advised by Coaches how to select models or what modelling can do, then SWO as Translators and step-in. Thus, no need to re-define the Translator role.

- **Is there a need to train translators?**

As evidenced by some of the impulse talks, the education of translators is very important.

- **Do you believe translation is automatable?**

87% of the audience answered with "No" (in conference poll). Irrational (emotional) decisions are taken at different levels within companies. Automation will not help/cannot enable this. Without enough data there is no AI (e.g., there is no or little data on how SME s can use simulation for their IP strategy)

Final remarks

The concept and practice of Translator is getting more established. Differentiation into more business and more technical oriented roles is ongoing and tools to support translators are in development.

Industrial needs on modelling tools for generating impact in industry and future game changers

Objectives

Identify game changers for industrial use of materials modelling in short- and long-term perspectives

Introduction

Industrial needs on materials modelling are a moving target since the requirements on industrial operations depend on changing regulation, market demands and overall policies (like Green Deal, Digitalization, etc.). On the other hand, completely new computing paradigms, like quantum and neuromorphic computing, show up which potentially will have a huge impact in the long term on industrial innovation processes.

The central question to be answered in this session is: Which features of modelling tools will change the game in industry in the near and long term from the perspective of identified industrial needs?

Discussion points and questions

- **Cloud computing, Quantum computing etc.: what's next?**

For the next generation computing Quantum Computing has the most attention, followed by neuromorphic computing. Material simulations are expected to be one of the first targeted areas for novel computing.

- **Digital Transformation, digital business models, new digital services lab of the future. Data based modelling, how to price and sell data? Standards and Ontologies**

There is still a lack of trust in machine learning/data-based models so physics-based models still have future. Industry is driven by costs when decisions are made. Such models need often extensive validation which means more costly tests. Models that are well developed and validated and show that can save costs will be very welcomed/needed.

- **Green Deal: green technologies/materials**

It will be key to produce new materials that are recyclable after the end of product life (cradle to cradle). This is very much of interest to a responsible consumer as they tend to think more about ethic and environmentally friendly products.

Final remarks

- Industry – Software - Academia Consortia enabled a most fruitful collaboration for both academia and industry for mutual benefits, i.e., academia developed a code with functionalities that were right away useful to industry.
- There has to be always an up-front investment by industry which comprises the cost of soft- and hardware and also their workforce has to learn to work with the software and invest time.
- New tools require re-thinking the approach to modelling as they enable not more of the same but different things to be done. That was true e.g. for linear scaling DFT and will definitely be the case for quantum computing based codes.
- Digitalisation looks as scientific modelling as one of four key areas also including data science, knowledge solutions (publications, patents etc) and digital laboratory/digitalised characterisation.

- It is important to achieve acceptance of materials modelling at the lab level. Integration of validated, reusable workflows into R&D digital platforms will be important to advance that.
- There is still a lack of trust in industry in machine learning/data-based models so physics-based models still have future.
- For the next generation computing Quantum Computing has the most attention, followed by neuromorphic computing. Material simulations are expected to be one of the first targeted areas for novel computing.

Policy

This Focus Area 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. It is aimed at assisting multiple stakeholders (Modellers, Materials Data Scientists, Software Owners, Translators and Manufacturers) that are 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.

EMMC Roadmap Strategy

Objectives

- Present the Roadmap implementation strategy and potential impact metrics based on a survey with H2020 coordinators (see Appendix A). Session participants will be invited to:
    - Identify further roadmap and implementation gaps and prioritize actions
    - Extend the reach of the implementation strategy by identifying synergies with other initiatives not yet connected to the Roadmap
- Community members involved in running R&I projects will share solutions to Roadmap deliverables and how they:
    - Address key market drivers of end-users and will generate quantitative Case Studies
    - Offer guidance to companies in developing their strategies with a translation approach based on existing materials knowledge and effective materials modelling
    - Improve the trust and credibility of materials modelling for industrial decision making for economic and environmental advantage

This Session aims to share anticipated Roadmap outcomes, proposed metrics for evaluation of successful implementation, and direction to communicate implementation success.

Introduction

The EMMC elaborates roadmaps that identify major obstacles to widening the use of materials modelling in European industry and proposes strategies to overcome them.

The EMMC Roadmap[4] is based on input from all stakeholders, including industry end users and materials modelling communities identifying gaps and actions to support the increased utilization of materials modelling in industry.

The Roadmap and its implementation address stakeholders from across the value chain, including modelers, materials data scientists, software owners, translators, manufacturers.

Three themes are emphasized in the Roadmap and are linked with R&I projects:

1. Development of Content: providing the *toolbox*
   1.1. Model development and validation
   1.2. Interoperability and integration
2. Development of the Framework for Deployment: making the tools readily accessible
   2.1. Data repositories and marketplaces: Materials Knowledge and Information Management
   2.2. Translation and Training for Companies
   2.3. Industrial Software Deployment
3. Implementation: creating industrial impact
   3.1. Tools
   3.2. Data generation, qualification and validation
   3.3. Processes
   3.4. Workforce Engineering/Talent Development
4. EMMC Roadmap Progress Overview
5. The EMMC implementation strategy for the industrial adoption of materials modelling was developed by consolidating input from materials and manufacturing industry members on what it means to achieve a mature state of adoption in their business environment, and their identified needs to reach that state. The current state of *maturity* was evaluated and categorized by *People*, *Tools*, *Data* and *Process*[5]. *Gaps* and high-level *actions* to reach maturity *targets* are summarized in Table 1 in relation to evidence of EMMC progress to bridge these gaps and current EMMC Focus Areas established to address key challenges in each category.
6. Progress against Roadmap implementation has been strongly evidenced with development of the Content (providing the toolbox) on topics related to model development and credibility. The community has promoted model and modelling workflow readiness through classification of modelling and documentation of simulation (ROMM[6] and MODA CWA[7]), and currently aims to implement ontology (EMMO) for enhanced interoperability across many material and process domains. Underpinning framework components included the *Open Simulation Platforms* (OSP) to promote accessibility to models and Business Decision Support Systems to link models with business decisions. Toolbox development will continue to be an underlying theme as adoption provides further feedback on gaps to reach maturity, and as new material and process topics require ongoing model development.

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[4] 2020, The EMMC Roadmap for Materials Modelling and Digitalisation of the Materials Sciences https://zenodo.org/record/4272033#.X7T1WHd2tpw
[5] Survey Template: Maturity of Materials Modelling
[6] What makes a material function? Let me compute the ways … Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology projects, 6th Edition, 2017, edited by Anne F de Baas. https://op.europa.eu/en/publication-detail/-/publication/e0845ae1-1b60-11e7-aeb3-01aa75ed71a1
[7] https://www.cen.eu/news/workshops/pages/ws-2017-012.aspx

7. Progress against **development of the Framework for Deployment** is active in current R&I projects in the contexts of establishing *Marketplaces*, *Open Innovation Environments (OIE)*, *Open Innovation Platforms (OIP)*, *Open Translation Environments (OTE)*, and relates to EMCC initiatives such as *Open Innovation Test Beds (OITB)* and *Innovation Commons*. The aim is to connect models, data, software, expertise, etc., for an enriched interconnection and promotion of available resources for industry access. We anticipate these activities will be deployed in the next three-to-five years, with the wider uptake of their strategies across multiple material and process domains. Figure 1 illustrates the connection between Roadmap deliverables and R&I projects and EMMC ASBL Focus Areas, and (we hope) indicates that there is extensive opportunity for implementation involvement across material/process/product domains. An indicative timeline of Content and Framework deployment is indicated by specific deliverables envisioned by the Roadmap over the past five years, in consultation with EMMC and EMCC stakeholders. Current and Target states were defined by the Maturity Model[8].
8. The Maturity Model encompasses both Content and Framework needs to assess the state of adoption of materials modelling by industry and will be updated in subsequent years. The Maturity Model is influenced by market forces and players beyond the control of the Roadmap implementation strategy.

Discussion points and questions

- **Of the actions discussed today in response to the EMMC roadmap, which one or two are the most pressing in the short term?**

Training and standardisation.

- **Are there gaps in the roadmap that we have not covered today that you think we should address?**

The gaps in the key topic "People" are:

1. Recognition and clarity or role(s) of modelling
2. Lack of Translators

The gaps in the key topic "Tools" are:

1. Integration of models: Coupling and Linking
2. Wider and better use of multiscale models
3. Model verification and validation

The gaps in the key topic "Data" are:

1. Fair data
2. Semantics
3. Data awareness
4. Analytics Capabilities

The gaps in the key topic "Process" are:

1. Business Integration
2. PLM integration
3. Value Chain integration

[8] White Paper: Strategies for Industry to Engage in Materials Modelling

Final remarks

To close the gaps in the Road Map, task groups may be spawned, and their outcome fed into a new roadmap.

The EMMC Roadmap in the R&I Landscape

Objectives

The objectives of the Session will be the identification of the EMMC Roadmap gaps related to different R&I funding programmes and proposal on recommended actions to fill them. The session will also be useful to raise awareness within the EMMC Community of the potential opportunities for funding their R&I activities.

Introduction

Materials Modelling and Digitalisation is a technology enabler to reach many of the policy goals targeted in the different EU programmes. In this session, funding programmes under preparation for the next multiannual financial framework (MFF) will be identified, where materials modelling and digitalisation has the role to foster innovation in companies.

A benchmark, of how these programmes are inter-linked with the EMMC roadmap priorities, will be performed, followed by gap identification and proposals for action (e.g., review of work programmes drafts and of EMMC roadmap).

In addition, synergies and coordination needs between the relevant actions in EU programmes will be explored.

Important background includes

- EMMC Roadmap[9], with six priority topics and recommended actions:
    - Model Development and Validation: improve accuracy and reliability, validation
    - Interoperability: ontology governance and support of tools; standards
    - Data repositories and marketplaces: digital hubs network, seamless services for industry
    - Translation and training: translation for SMEs, training in the diverse aspects of materials modelling and digitalisation
    - Industrial Software Deployment: support European software industry and its underlying base.
    - Industrial Integration: support acceleration of maturity growth in industry
- Proposal for a REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL[10] establishing Horizon Europe, September 2020
- Political agreement on the 2021-2027 Multiannual Financial Framework (MFF)[11], December 2020
- Horizon Europe[12]
- Digital Europe Programme[13]
- European Defence Fund[14]

[9] https://emmc.eu/activities/emmc-roadmaps/
[10] https://www.consilium.europa.eu/media/45766/st11251-re01-en20.pdf
[11] https://www.europarl.europa.eu/RegData/etudes/BRIE/2020/659371/EPRS_BRI(2020)659371_EN.pdf
[12] https://op.europa.eu/en/publication-detail/-/publication/eef524e8-509e-11eb-b59f-01aa75ed71a1
[13] https://digital-strategy.ec.europa.eu/en/library/digital-europe-more-competitive-autonomous-and-sustainable-europe-brochure
[14] https://ec.europa.eu/growth/sectors/defence/european-defence-fund_en

Discussion points and questions

- **Which of the six EMMC roadmap priority topics (see above) seems to be better addressed by the R&I funding landscape?**

The six priority topics will not get explicit funding. The EMMC will have to closely follow the Horizon Europe Clusters and position the six priority topics as enablers, i.e., with BETTER …

1. Model Development and Validation
2. Interoperability
3. Data repositories and marketplaces
4. Translation and training
5. Industrial Software Deployment
6. Industrial Integration

… we are ENABLING …

… to build a competitive, digital, low-carbon and circular industry, ensure sustainable supply of raw materials, develop advanced materials and provide the basis for advances and innovation in global challenges to society. (Cluster 4: Digital, industry and space)

… to fight climate change by better understanding its causes, evolution, risks, impacts and opportunities, and by making the energy and transport sectors more climate and environment-friendly, more efficient and competitive, smarter, safer and more resilient. (Cluster 5: Cluster 5: Climate, Energy and Mobility)

The Digital Europe programme offers 7.58 billion for:

- High Performance Computing (€2.2 billion) – relevant to EMMC topic 1
- Artificial Intelligence (€2 billion) – relevant to EMMC topic 2
- Cybersecurity (€1.6 billion)
- Advanced digital skills (€577 million) – relevant to EMMC topic 4
- Ensuring a wide use of digital technologies across the economy and society (€1 billion) – relevant to EMMC topics 1-6 as they are all needed to enable a wide use!

- **Which of the six EMMC roadmap priorities seems to be poorly addressed by the R&I funding landscape? What actions can be done to improve that situation?**

None. It will be up to the EMMC community to advocate these priorities at any given opportunity.

- **What have been the main challenges or limitations identified so far in H2020 by the EMMC community to better implement the roadmap?**

  What is needed is to …

  1. Track, promote, quantitatively assess the progress of the EMMC Roadmap solutions developed in R&I projects
  2. Use, refine, create tools for quantitative assessment for materials modelling
  3. Consider a common approach
     a. Aggregate impact statements across projects to promote solution benefits
     b. Improve integration with business
     c. Collaboration with existing, integrated solutions (commercially established)

- **EMMC and EMCC (modelling and characterization councils): how should they cooperate going forward? Is it better to keep two councils or should there be a one in the future?**

Two councils with close links as both have a responsibility to cater for their particular community. To enable these actions in Horizon Europe, there is a need to establish a closer collaboration on actions between EMMC and EMCC to enable these actions, and to identify industry needs and challenges.

- **Which actions would you recommend to EMMC community to better align to the policy priorities?**

A focus group each to establish, how a policy can enable the objectives of the R&I funding landscape. By doing so, the EMMC community will naturally enhance their assets.

- **Which are the potential synergies between the different R&I programmes in terms of advanced materials and materials modelling?**

All programmes require "better/different materials". Materials Modelling has proven itself to be useful. Hence, the EMMC community needs to be vocal and present when the time comes to join this project. They have to be proactive and bring all the benefits of Materials Modelling to the table.

- **How can the community best contribute to the challenges, needs and opportunities outlined in the talks? For example, regarding Green Deal, Critical Materials, Quantum Computing etc.**

All opportunities are given. The EMMC community will have to elaborate how their common skill set can enable these challenges.