The European Materials Modeling Council

EMMC Survey of materials modelling development needs: discussion notes towards the Road Map 2018-2020

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Impact of materials modelling in industrial sector

The impact of materials modelling on the industrial sector is clarified by:

- The increase cost of developing a 21st century product with its prerequisites, requires a smart goal-seeking design procedure where a performance-based (back-engineering) functionality of the product is guaranteed.
- Virtual integration of processes will reduce costs.
- Materials modelling is already part of many business processes but it can become a more impinging part if the economic advantage for the end-user becomes clear.
- Majority of managers (in SMEs) are not aware of importance (and what a difference can be achieved) of a proper material selection and material sourcing to deal with the quality and functionality on one side and the costs on the other. The awareness and training as well as the market place would be important.
- Minimize expenses and time needed in achieving a functional and marketable end product.
- What would be interesting would be to become able to select the proper model for given manufacturing problems. For example additive layer manufacturing is an area where material modelling is essential, but where the physics of the phenomena is poorly understood, through the scales, and through the production process itself.
- To increase impact connecting with Industry 4.0 is crucial, and developing process to end user (material performance) workflows and toolsets is critical.
- Virtual factory models would revolutionise manufacturing. Requires level of IT expertise way beyond that of traditional modellers; partnerships are vital here for upscaling of materials models to include databases towards development of business decision making software tools.
- The impact of Industry 4.0 is well known and at least the main goal of all our action. Modelling along processing and manufacturing is the digital key for innovation and thus, has to be crucial part of coming research action.
- Materials discovery. To use theoretical methods and modelling to propose novel functional materials and motivate further experimental work. The benefits of such activity for final business value are probably long term (> 10-15 years), but a thoroughly designed road-map towards theoretical discovery of new materials might help to accelerate the implementation of future revolutionary materials. To this end, efforts on the development of

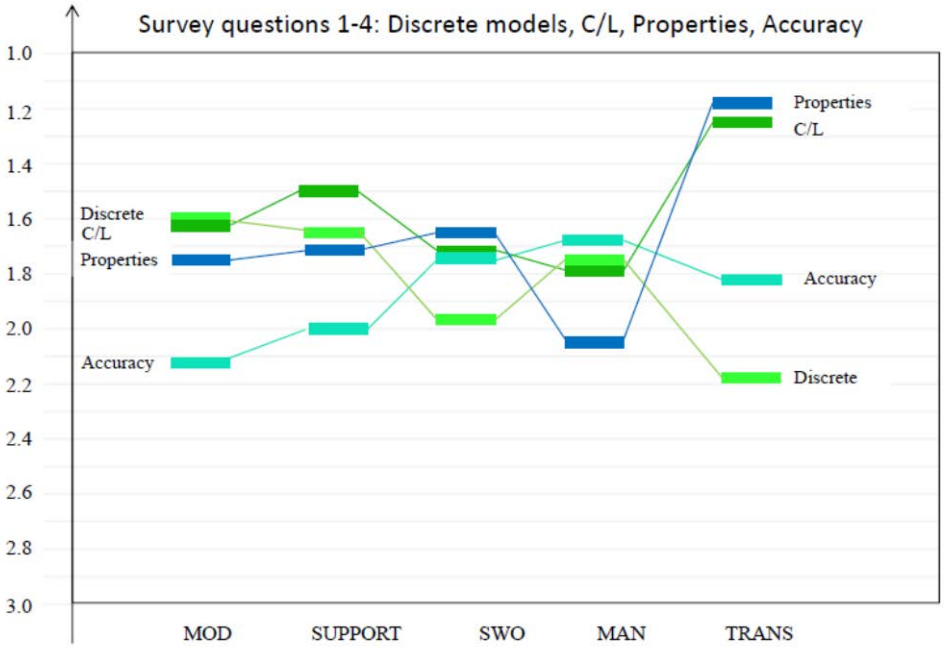
new structural search engines, structure-properties descriptor analysis tools, and efficient workflow schemes are needed at this stage.
- Reducing variance in a chemical product. Improving analysis why the variance is taking place.

Section A: Motivation of this survey and collected analyses

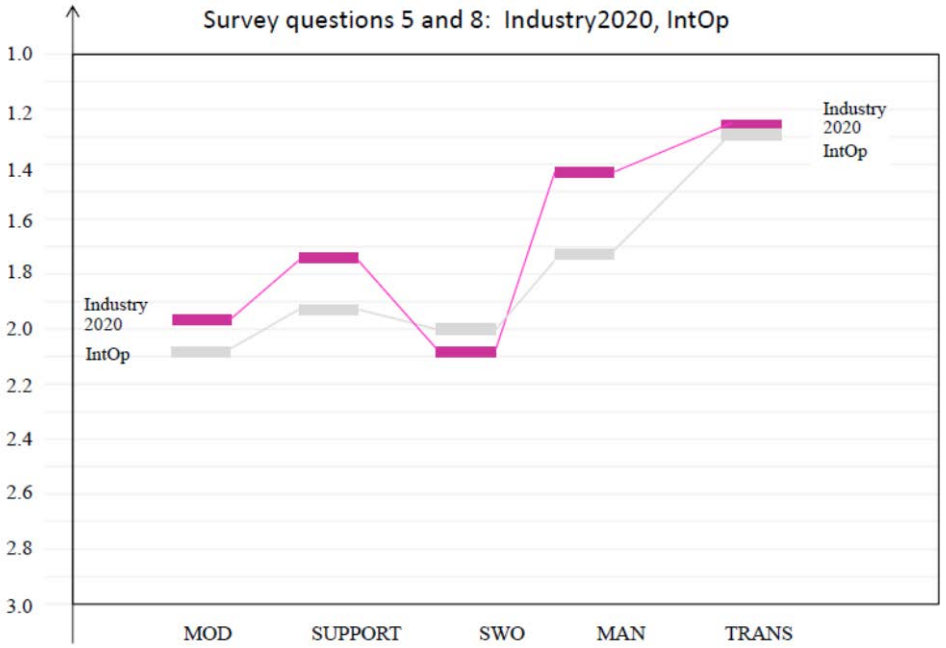
During the last two years, EMMC has worked in defining the most relevant actions urgently needed for promoting further the use of materials modelling in the industrial sector, thus making the previous expectations real. However we have felt the need to consult systematically a larger set of stakeholders and hence we have designed an online survey about materials modelling needs. More than 1500 stakeholders were invited to fill in this survey and we elaborated by feedback of more than **250 participants (20% are manufacturing industries and 40% software owners)**. This survey largely confirmed the most critical actions identified by the EMMC, but it also provided new ideas which will be used as a basis for discussions towards the Road Map 2018-2020. We asked each participant to rank each topic in the range 1-5 (1 being the most important) both in terms of importance and urgency of the topic. We assumed 6 for those who did not reply about a specific topic. In the following table, the topics are reported in the decreasing order with regards to the product of importance and urgency, used as in indicator of the relevance of the action, namely **Relevance = Importance x Urgency**.

	Importance	Urgency	Importance*Urgency
Coupling/Linking	2,13	2,19	4,67
Discrete models	2,21	2,35	5,18
Properties	2,25	2,45	5,51
Industry2020	2,45	2,55	6,25
Accuracy	2,52	2,63	6,62
CSA	2,74	2,80	7,68
IntOp	2,74	2,81	7,71
MMP	3,15	3,21	10,10
BDSS	3,14	3,26	10,26

Some comparative analyses of the collected feedbacks are reported next.



The graphs show the average score for each stakeholder group. Individual answers were in the range 1 - 5 (with 1 highest). The results were exported from the web survey on 5 May 2016. Analysis by KH.



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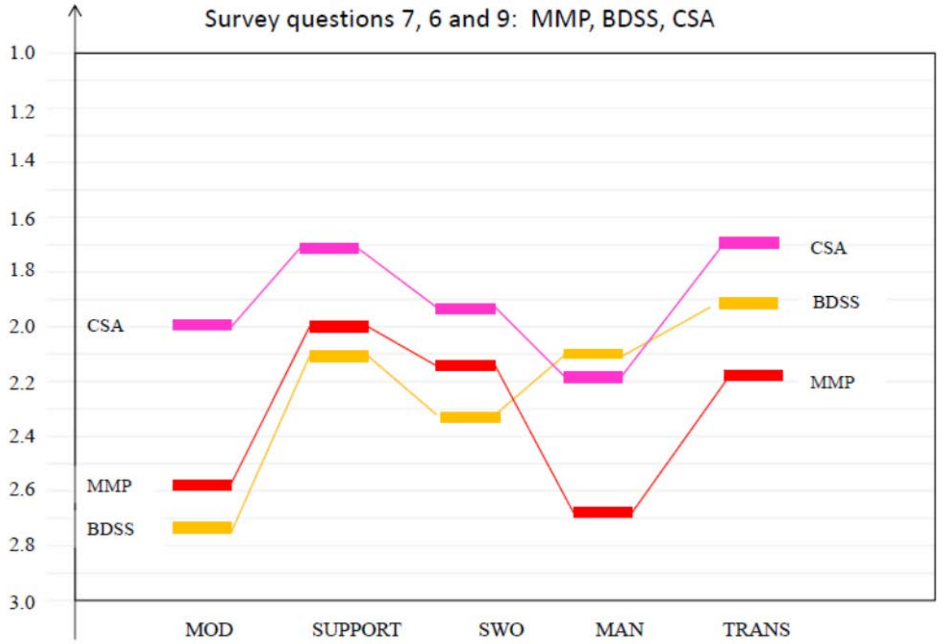

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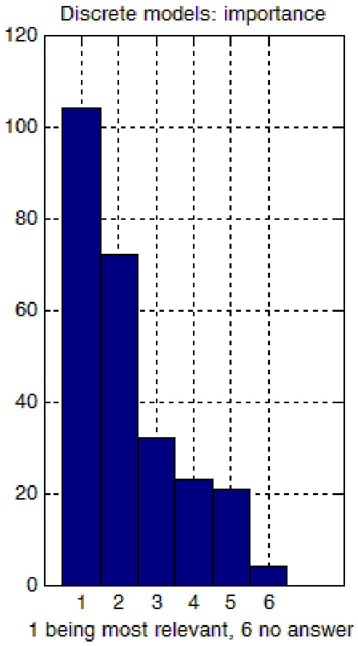
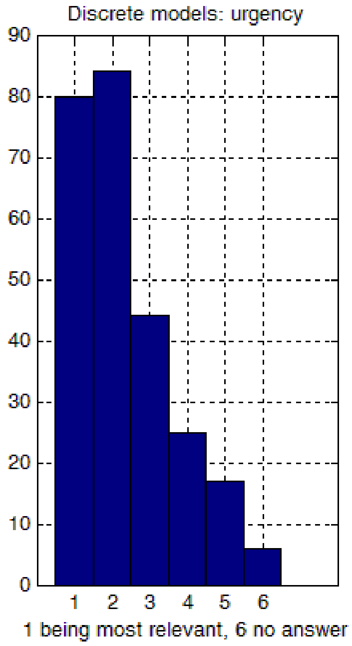
Section B: Materials modelling development

(1) Materials model development: Enhancing the use of discrete models (electronic, atomistic, mesoscopic)





Discrete models received a high priority score among all the stakeholder groups. Almost all of the participants in the survey listed one or many fields where the currently available discrete models are insufficient or lacking and hence model development is needed. Both predictive and qualitative model needs were mentioned, with a focus on the need for models to handle large and complex systems, such as multimaterials, complex composites and interfaces of different kinds. The lack of good atomistic force-fields was mentioned in many answers. A very broad range of application fields were mentioned, from electronic materials to crystal growth to catalytic phenomena and solar cells, packing materials, soft matter, nano- and biomaterials and medical devices, to name a few.

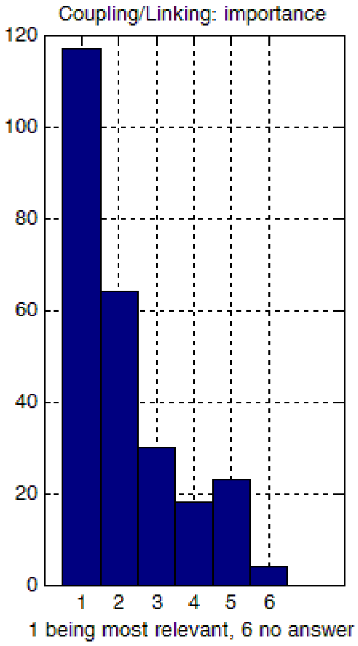
Several members, including the manufacturers group, used words like *new insights*, and *enhanced understanding* in their description of the need for discrete model development. A respondent from a research institute wrote: *"From a research institute point of view [discrete] models are invaluable to provide us with insight needed to serve the industry."*

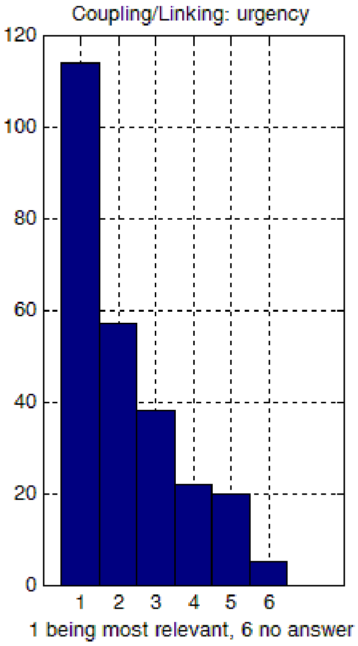
Strong needs for improvement of workflows (or "methods" as the responses usually said) were also expressed. A need that stands out above the rest, is workflows that enable long time-scales, large systems, rare events etc. to be explored, an issue that is of course coupled with the model development need.

(2) Materials model development: Enhancing coupling and linking

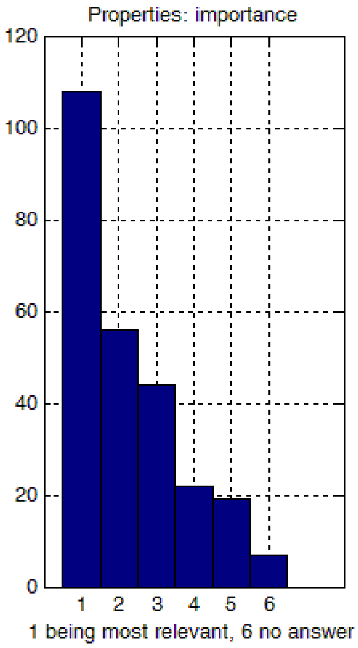
This topic has a high priority among all stakeholders. It is seen as a promising vehicle towards realistic modelling of applications of industrial interest, although the complexity and challenges of the topic are fully recognized. The survey answers given exemplify a broad range of areas where a strong need for development of such C/L (multiscale) models has been identified. Model-wise, C/L needs among the discrete models are listed as well as between discrete and continuum models, and between various flavours of continuum models. Both top-down and bottom-up approaches for materials design, property calculations are process simulations are mentioned.

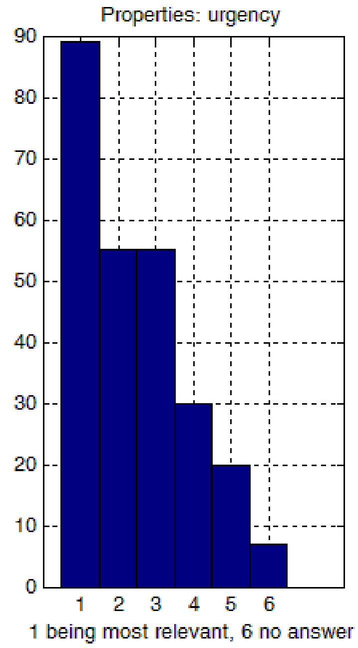
Here not only challenges in terms of the model-focussed efforts, i.e. the strategies to select what degrees of freedom to dispose of (or add) in the coupling and linking process, are highlighted in the comments, but also the need for activities related to automated, accurate linking workflows, standardization of data exchange formats, and the development of friendly linking platforms generalized software frameworks etc.



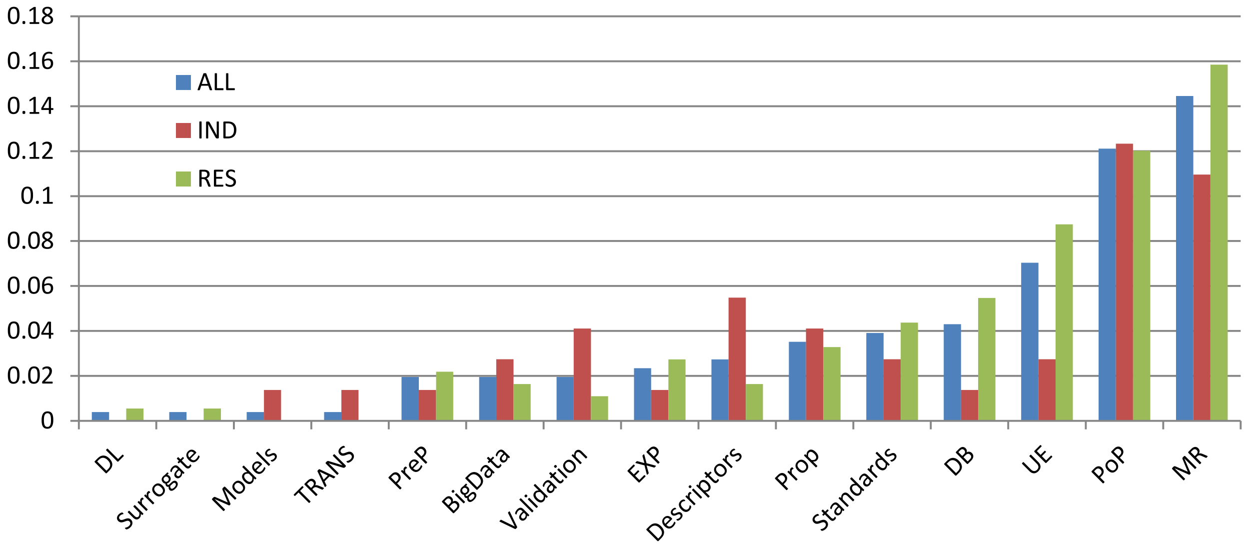


(3) Extracting materials properties from models





The free text was manually scanned to identify the main keywords in relation to the RoMM and using the RoMM as a language reference. In total about 17 distinct keywords were identified for Industry 2020. The following histogram shows both the keywords identified from the analysis of the free text and the resulting distribution for all stakeholders (all), industry only (ind) and research (res). Note that the plot is the relative percentage from with respect to all, Industry and Research, including those who did not provide any input.



DL: Deep Learning, Machine Learning.

Surrogate: approximate models.

TRANS: need for translators to define the properties.

PreP: general pre-processing.

BigData: analysis of large sets of properties.

EXP: estimate properties that can directly be related to experimental characterization.

Descriptors: include KPIs and sophisticated properties that determine the overall behavior of a material.

ProP: general property calculation, multiple fields were mentioned ranging from thermodynamic, mechanical macroscopic properties to rheology of complex fluids and diffusion.

Standards: standardization of the calculation of properties.

DB: support databases of properties.

UE: supporting the uncertainty estimates in properties.

PoP: general Post processing, without specifying to which application or which specific actions that need to be made.

MR: refers to on-the-fly material relations that are extracted from one morel and used in another, especially from discrete to continuum.

Stakeholders understanding of this category varied between two extremes: those who think this is a simple technical task which does not require any additional thoughts to those that saw it as an important part of the modelling workflow that is the least developed!

What is noteworthy is that most stakeholders see the role of extracting material properties as part of the coupling and linking workflows. For this the keyword category MR (Material Relation) was chosen. In this sense a MR is simply a mean to move information from one model to another. Most stakeholders refer to extracting material properties to couple discrete (especially atomistic) to continuum models as especially needing action. In this sense the MR is to be seen as a derived property from one model to another, alleviating the need to use phenomenological MR. Especially the development of force field and interatomic potential databases was also highlighted in the feedback and is included in this category and the DB one.

The second category that was identified is Uncertainty Estimates. To this category all feedback relating to either quantification of errors or predictability of any sort was adjoined. Validation, which effectively belongs to this category, too was left alone since many stakeholders distinguished between it and UE. If we sum the feedback relating to UE, Validation and EXP, which means getting material properties that are comparable directly with those obtained from experiments, then we can identify clearly another action (validation) as summarized below.

It is also interesting to note that many stakeholders would like to see databases and standardization efforts going in the direction of calculating these properties in a pre-defined manner so that properties calculated using different methods can be compared straightforwardly.

The notion of descriptors (which includes KPIs and getting meaningful parameters) is another important point needing action.

Post-processing in general was highly evaluated as needing action as well. In this sense, there is a need to direct some efforts to projects that include the development of methods, and models from to post process the data, however the feedback here should be seen as too general, and is in fact covered by the other categories needing action listed below.

Another interesting point is the need for special HPC property estimation for high throughput calculations, Deep Learning and Big Data (all lumped into Big Data, except when DL was explicitly mentioned).

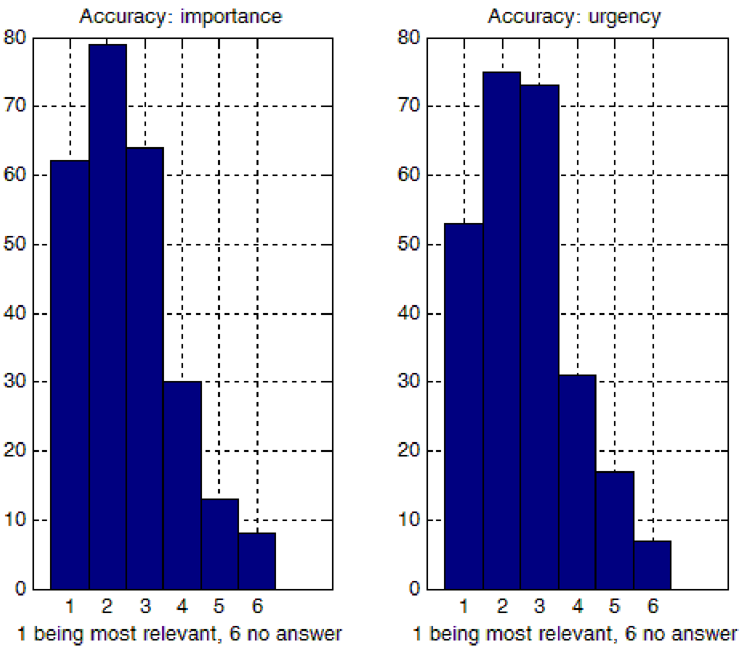
What is quite surprising is that preprocessing took a low priority, however each post processing step is in effect a preprocessing step for the next step in the workflow, so both are connected.

In summary the following actions are supported by all stakeholders:

1. Extracting properties for coupling and linking between models (MR)
2. Validation and UE of these properties so that comparison with experiments can be made, facilitating the integration of experiment and modelling in the same workflow.
3. Development of sophisticated descriptors and KPIs
4. Development of rapid extraction of properties for Big data analysis and machine learning (deep learning).

Industry in particular highly ranks Descriptors and Validation of post processed properties. In other words the ability to extract reliable information from the simulations that can be directly used in business related workflows is needed by industry.

(4) Extracting the accuracy of different models



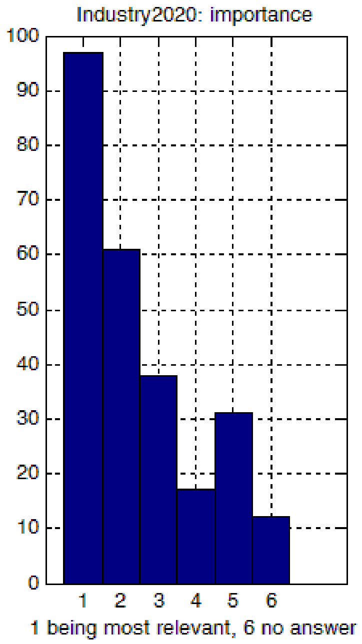
A majority of the responses comments state that this topic represents an important and even crucial area. Getting a handle on, and improving (see question 1), the model limitations appear to be a prioritized issue among all stakeholders.

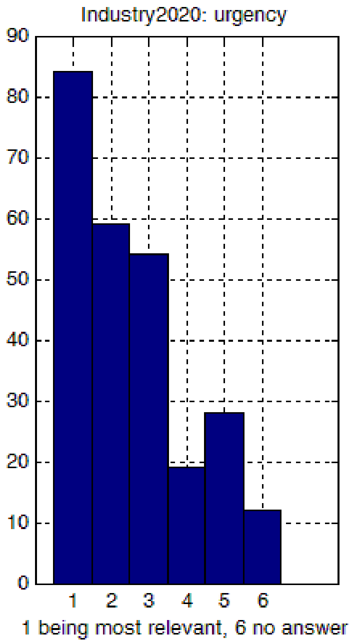
It is also clear from the answers that model assessment and error quantification exposes many facets, where for example, predictability is not necessarily the sole, or main, goal in terms of accuracy. Achieving a reliable direction, a qualitative trend, may be the. Thus among the manufacturers, several expressed that reliable qualitative trends derived from modelling are useful, while predictive quantitative data may be the ultimate goal. In either case, assessment of the accuracy/uncertainties/limitations/errors of the model results is crucial to help designers and manufacturers make the correct selections. For example, knowledge of the relation between calculated materials properties and model parameter was high on the list among some respondents, while others suggested the launching of large-scale benchmarking projects to facilitate assessment. Overall, validation with the help of experimental data was emphasized in a large number of answers. A few raised the point that a main obstacle here is the uncontrolled conditions of most experiments.

It was pointed out by many respondents that *accuracy* can be an ill-defined concept, as one and the same model can be either accurate or unprecise depending on how it is applied. Here the remedy can lie in the inclusion of more of the relevant physics contents for the application at hand.

(5) Integration of materials models with manufacturing and processing (Industry2020)

The free text was manually scanned to identify the main keywords in relation to the RoMM and using the RoMM as a language reference. In total about 17 distinct keywords were identified for Industry 2020.





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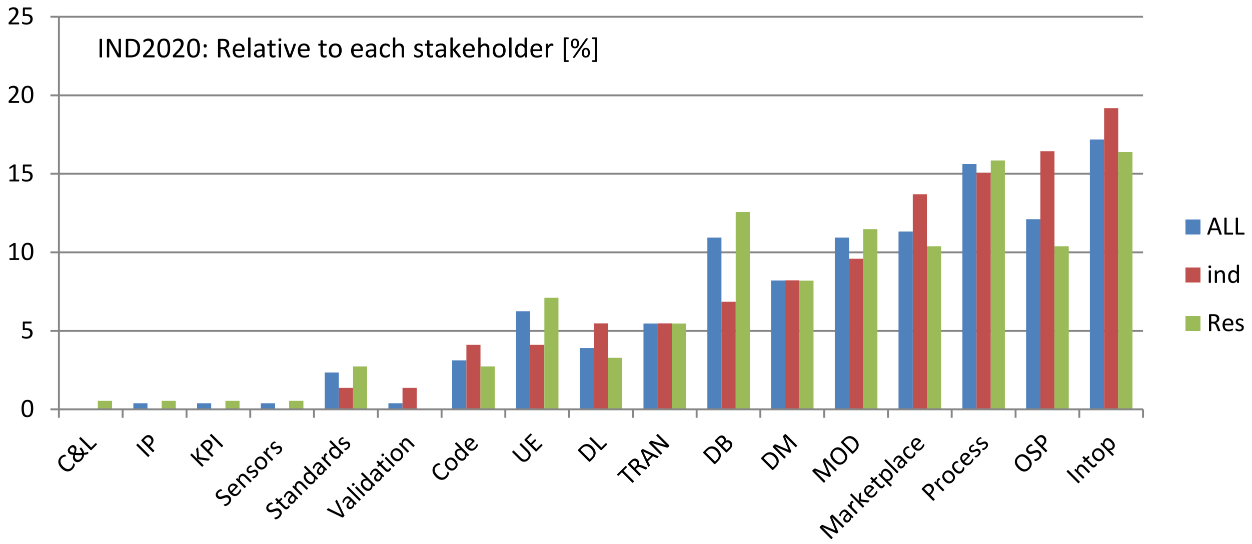


What is surprising is that there is a correlation between the distribution of research and industry, reflecting a common understanding on the topics of importance.

IntOP: This refers to the interoperability between simulation and characterisation, i.e., how to integrate both simulations and experiments into the same workflow. This includes also coupling of hardware and software systems in the same platform. In addition the integration of characterising (online, and offline) with materials modelling workflows was also highlighted. Databases of characterisation data as well as modelling data have been numerously highlighted. The need for interoperability between simulation tools and characterisation systems was also noted highly.

OSP: This reflects the need to integrate and couple both experiments and simulations into a common platform necessary for industry 4.0. This category is of course related to the IntOP as integration into the OSP requires interoperability between the tools. Also workflows, standards for data and models as well as experiments and standard pre and post processing enter in this category.

Process: Another major keyword which reflects the need to model and take into account the whole process chain, from the material selection down to processing and final properties and vice versa. In this context, KPI as a means to identify key parameters affecting the design and final product properties was mentioned. The need to integrate Sensors and includes pre and post processing is also included in this category as it is essential for the description of the process.

Marketplace and Databases: many expressed the need for a web based platform that provides integration of all components needed for the process description including both experiments and modelling. Both databases of modelling and characterisation are included in this category.

MOD: Many expressed the need for better more accurate models in order to be able to describe the system and process reliably. Especially advancing the predictability of models, in particular discrete ones and their integration with continuum models was highlighted. Additional important points are more accurate and approximate faster models that can be integrated with experiments.

Translation: Translation What is also surprising is that many have expressed the need to better translate modelling to industry and to better explain the benefits of modelling as a prerequisite for industry H2020. This includes rising awareness for capabilities of models, education and training as well as helping the industry to choose the right components in their industry 4.0 related workflows.

Digitisation of Materials: In this context a need for describing and managing the whole process data was highlighted including the processing history.

Validation and UE: Though Validation itself was not addressed often, the Uncertainty Estimates (UE) belong to the same category, and have been highlighted as important factors .

Code: what is also particularly interesting is the need to develop faster more efficient codes that can deliver information in a rapid and efficient manner to enable tighter integration with characterisation on the production line and faster solution to problems. This includes Extreme Code, faster modelling, numerical methods.

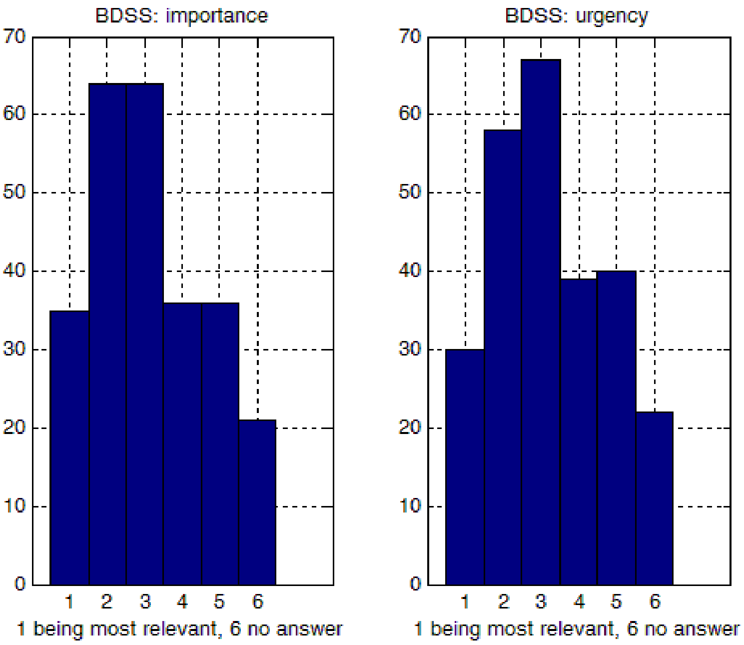
DL: Deep learning which included Artificial Intelligence and data analytics was highlighted.

(6) Integration of materials modelling in business processes

The free text was manually scanned to identify recurring topics which are summarized below:

Impacts to be expected

- Upscaling and market introduction with **increased speed and reduced risk** (Using modelling to target key risk factors, ability to make fast adjustments due to integrated materials modelling, etc).
- Virtual integration of processes will **reduce costs.**
- **Minimize expenses and time needed in achieving a functional and marketable end product**
- This is already occurring in the materials for nanoelectronics, the most advanced manufacturers are investing in this area. It is difficult to quantify a financial impact as the main objective is to **narrow the selection of potential materials and to reduce cycle times**. In many instances, it is not conceivable to design products without these tools for support.



- I would expect in the not so distant future simulation will be a basic **tool of exchange information between the different departments in industry**. And will serve as an **education and promotion tool for products or processes**.
- Enhancing possibilities of direct application of numerical modelling in Knowledge Based Systems (decision-making support systems). Developing capabilities of 'material design on demand'; Knowledge Based System with modelling tools is able to suggest the best (or a set of good-enough) material for particular technological demand. If any available, **suggest direction of new material development**.

Estimation and Quantification of Impact

- The **quantification of the impact** regarding materials modelling in industry; **financial data and multi objective optimisation toolboxes** are all very important actions for the integration of materials models into business processes.
- **Indicators for evaluating the impact** are needed.
- Calculation of cost reduction of cases with and without materials modeling (less trial-and-error, less hardware designs, etc.). Especially enabling quantitative and objective

comparisons between the 'virtual' (modeling) and 'physical' (laboratory) development cycles for specific devices/products is extremely urgent.
- Better estimate of overall cost of modelling is needed.

Challenges and requirements

- The big challenge is to combine models not designed to communicate with other in a useful way. This **requires robust semantic interoperability schemes.**
- Novel **artificial intelligence models** for the combination of models (discrete and continuum) for structure-function-process optimization.
- To increase a substantial interest and enthusiasm about the possibilities for virtual product development, **a more smart computationally oriented technique is required**. The increased cost of developing a 21st century product with its prerequisites, requires a smart goal-seeking design procedure where a performance-based (back-engineering) functionality of the product is guaranteed.
- The integration of **"context" data** will be in the future a key for competitiveness and process optimization.
- **Certification** of materials models for industry use
- **Standardization** is, in our opinion, the key to enable a proper integration of material models with manufacturing and processing.
- Industrial and business processes should be **digitalised** as much as possible with fully integrated material models.
- Support (organizational and financial) for spin-outs providing **modelling services** for industrial sector.
- **Industrially relevant properties and KPIs**

Need for improved dialogue, collaboration, transparency and coherence

- There is no proper dialogue, connections and understanding between those dealing with the materials modelling, industrial designers, innovators, industrial processes and the business managers.
- Some guidelines or case studies for an individual industry or sector (also in the form of infographics, graphically presented process flow or similar) in this fields would be useful to the future call applicants as well as to all those who would like to become familiar with the subject.
- Majority of managers (in SMEs) are not aware of importance (and what a difference can be achieved) of a proper material selection and material sourcing to deal with the quality and functionality on one side and the costs on the other.
- Materials modelling doesn't have answers to all of the problems, so all of the stakeholders need to be clearly aware of this fact. Effective communication should help to optimize efforts/time and efficiently combine available resources and working teams.

Use cases

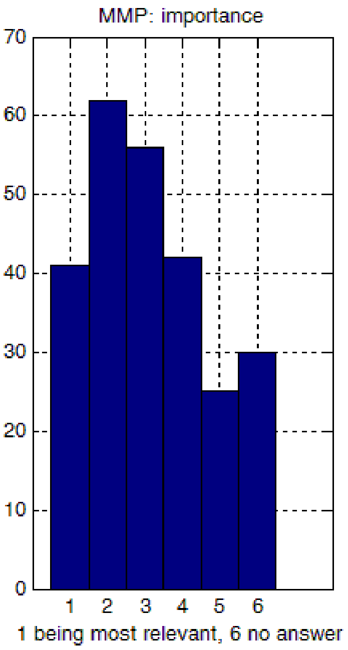
- The urgency must come from particular use cases for industrial- business- people.
- Availability of previous application cases and success history (if any) and make available and easily accessible comprehensive data on available patents.

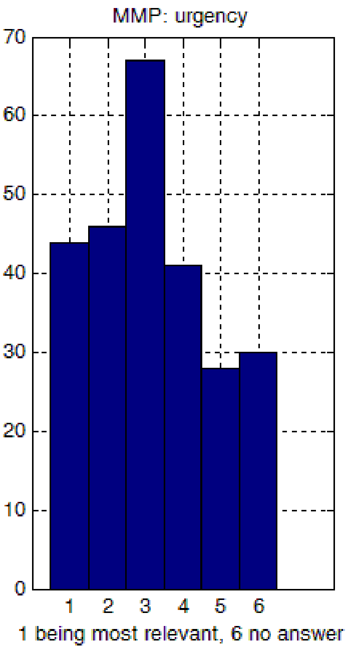
- I think this will happen naturally once we have a good collection of case studies demonstrating the return-on-investment with the adoption of multiscale modeling

Neutral/Negative

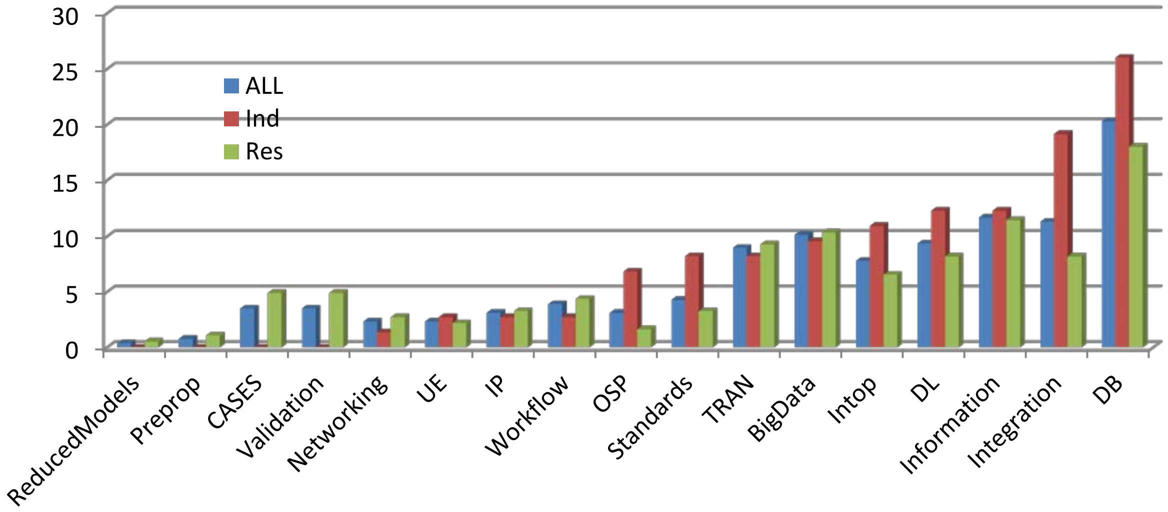
- Material property modelling tools will have significant industrial impact, as many manufacturing industries are essentially converting materials to standardized microstructure, properties and performances. Material modelling tools will enable manufacturing industries to innovative products formulations and structure more efficiently and faster. However, I do not see the need to integrate material modelling in business processes.
- Not as important as the other parts. Big company know how to deal with the results they obtain as long as they are aware of the accuracy of the predictions
- The tools are not mature enough.
- This topic is usually driven automatically by material suppliers and does neither need governmental guidance nor any kind of support.
- Again, it is a question of readiness and reliability which may vary across the industries. I do not see feasibility of integrating the material modelling into business processes, apart from the marketing.

(7) Materials modelling Market Place and dataspaces



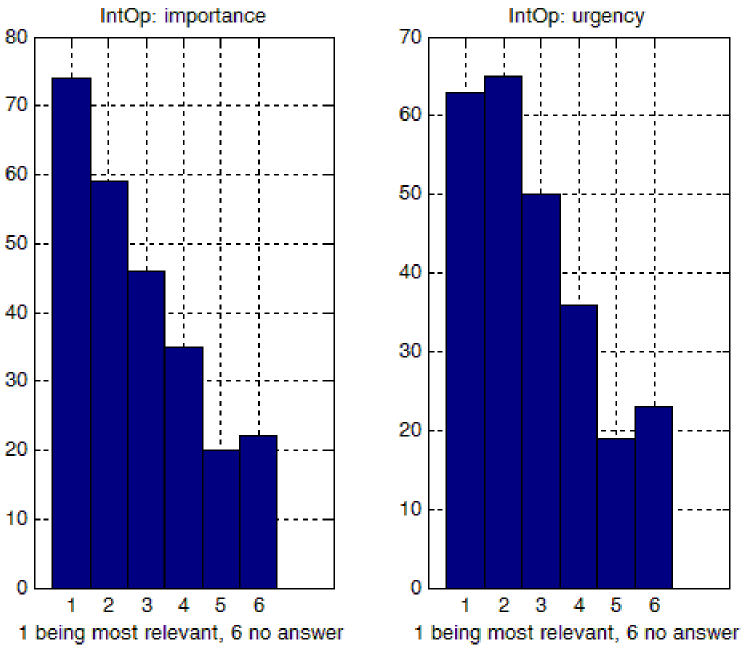


The free text was manually scanned to identify the main keywords in relation to the RoMM and using the RoMM as a language reference. In total about 17 distinct keywords were identified for marketplace and dataspaces.



In the marketplace there is a strong need to support information management and exchange in an open way that still preserves IP rights for industry. Databases and integration of workflows is a dominant factor. Perhaps surprising is the need for Bigdata analysis and Deep Learning (including Analytics and artificial intelligence methods) in the Marketplace platform. The databases and integration are seen to be highly ranked by industry. In fact if we sum the input for integrating, IntOP, and standards as well as OSP, almost one third of industry highly regards integration with Databases taking second place with 20%. Industry is also seen to be more keen for standard interfaces and interoperability that research.

(8) Integrated workflows and interoperability including experimental data



- Semantic interoperability in materials modelling
- The big challenge is to combine models not designed to communicate with other in a useful way. This requires robust semantic interoperability schemes.

- Businesses require the lowest cost for a specific purpose. The choice of material is part of that and better decision support systems for materials are needed.

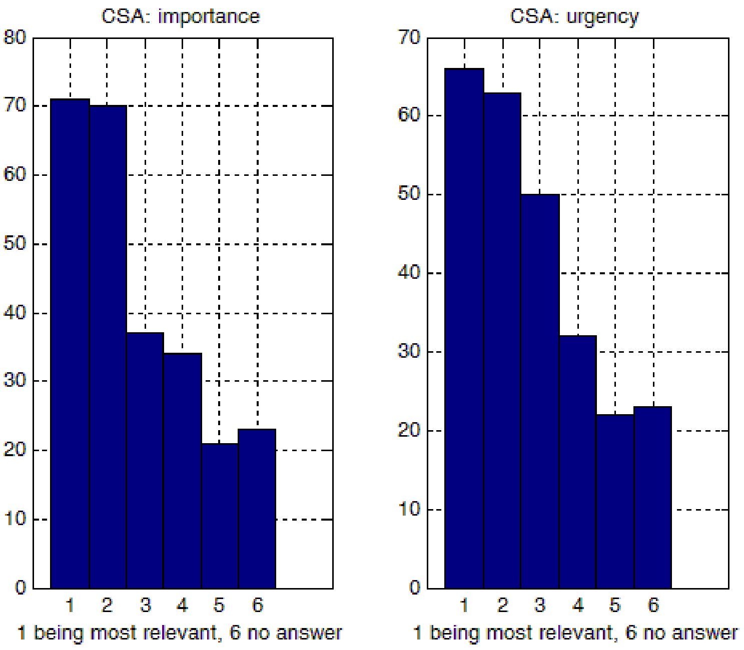
(9) Coordinating network: Enhancing the uptake of material modelling by Manufacturers

The community replies can be in short summarized with the activities of EMMC:

- Wide stakeholder consultation,
- Stimulate complementary activities to what already exists,
- Stimulate exploitation of existing materials modelling expertise in industry,
- Stimulate model development necessary for industrial applications,
- Provide inputs for EC future visions/plans.

There were many similar replies from experts; just excerpt (in order avoid the repetition) is given:

- Continuation of the EMMC CSA would be of immense importance,
- Enhance the networking and communication between all existing modelling communities, with more links to industrial materials producers,
- Not only transfer the knowledge from academic to industry but also vice-versa: a clearly defined need of models coming from industry,
- It is important to show stories of success. This requires support to develop multiscale models for industrial applications,
- Provide and start from simple solutions/cases and killer applications that manufacturers will feel as a real gain and benefit,



- Coordination network is the only way to arrive at broadly adopted standards, which in turn will lead to automation of workflows,

- Wide stakeholder consultation to try to change perceptions and the culture in industry about simulation and its benefits and cost-saving potential,
- 1) Continuation and reinforcement of coordinating platforms like EMMC or ICME are highly beneficial coordination network to focus on 'interoperatibility' of models 2) Undertake further and more activities to also include new generations of future participants, users, decision makers from early training stages onwards, e.g. students from universities 3) special workshops, info platforms or online media tools for interested manufacturing industry members or employees, e.g. by using successful example case studies,
- One of the main features of the simulation systems for manufacturing processing is to setup a smart modular framework to employ a proper material model for different stages of manufacturing and service life. The extent and limitation of models and their length\time scales which have to be spanned to reliably simulate the material behaviour should be determined first, and the appropriate modules should then be employed to carry out the material simulation,
- Already proposed topics within EMMC provide a good venue to cover up these points,
- The communication between disciplines and existing especially national networks should be improved. There should be a complementary and well aligned EU action which studies differences and which defines adequate interaction in order to focus on the same goals,
- Multidiscipline networks help material modellers appreciate the fabrication and product design difficulties while manufacturers appreciate the scope of available models and help to identify the existing gaps (stimulate complementary activities to what already exists),
- Stimulate exploitation of existing materials modelling expertise. The best idea is not valuable if manufacturers do not adopt them,
- Networking of modelling communities in order to spread new methods for analysing different phenomena and to extract material properties from models,
- Enhance the training on modelling in the manufacturing community,
- Stimulate model development necessary for industrial applications - enhance the transfer of models from academy to industry and software owner,
- This appears to be a realistic and important goal for the near future. Increased awareness and collaboration with industry can serve as a good stepping stone for further actions. It will give practical aid to European industry with a foreseeable positive outcome in the near future. Enhancing the transfer of model development from academy to industry and software owners deserves support in actions,
- We need to strengthen existing networks and facilitate the current communication among different stakeholders. Broader networks/meetings are needed: less specialization on particular fields, but more focused on open challenges and how to face them from multi-faceted perspectives,
- More use of modelling in industry would lead to the improvement of product quality and integrity, tooling and process optimisation, energy conservation, reduced emission and cost reduction - to ensure sustainable manufacturing,
- Establishment of a network linking end-users and modellers - Getting more involvement of manufacturers in setting development and innovation priorities, this would imply also obtaining funding from manufacturers for specific actions. Perhaps the creation of a PPP in this area could be useful to put in contact these two communities and to provide additional funding to stimulate,
- Networking is important, but more important is in my opinion that these networking activities are continuous,
- Identification of barriers to uptake of materials modelling by consultation with those who are not using these models. Promotion of the benefits of materials modelling to resistant communities

in a language they can understand. Guidance for academic model developers on how to talk to industrialists about materials modelling,

- Introduce modelling basics in all Engineering education Europe wide Organize free, open access, databases that ensure the anonymity of the users,
- The coordination of networking and financial support are necessary to translate and exploit the material modelling value from academic, to centre research, to industrial end-user. The methodology and software are the tools to exploit the potential of materials models in easy, friendliness and flexible way,
- Coordination network would support uptake of high quality open-source models by industry,
- Estimation (quantification) of the impact regarding the materials modelling in industry is the key point. Then Networks to advance the update of materials modelling and stimulate model development necessary for industrial applications,
- No systematic periodical survey from software development companies seems to be performed or proposed to all users and/or customers. This kind of survey could be useful to users to understand enhancements at each software release,
- The most urgent action is in my opinion to stimulate the exploitation of existing materials (and process) modelling expertise,
- Estimation of the impact of complex material models in industry real cases of application. Promoting the use of advanced material models that are multiscale and multiphysics in industrial cases,
- Enhance communication between academia and industry: dissemination actions, joint workgroups, joint regular publications, industry PhD's, etc... - Improve oversight of material models development by manufacturing stakeholders,
- CSA or RIA actions are necessary for the advance of material modelling and for the transfer of knowledge from academic to industry. In particular, an action is needed to support the establishment and the upgrading of a Simulation Platform dedicated to the interoperability of models and tools. This support is fundamental to guarantee its reliability in addressing the industrial needs,
- Creating and supporting a business model for even closer collaboration between both modelling and experimental research communities and industrial companies. Creating a one-stop market place for (1) finding existing modelling solutions, (2) finding or requesting measurements of materials characteristics, and (3) finding or requesting specific contract work carried by academia for industrial companies,
- Transfer of competence from institutes & universities to companies. Standardisation of interfaces of software. Clear documentation about models, test data, and its meta-data. Robust models,
- Enhancing the transfer of models from academy to industry, Experimental validation of predicted behaviour of industrial products.

(10) Are there any broad areas that we are missing?

- Set up of university- and industry-level **training** courses on materials, process and performance modelling. Development of adequate training tools and case histories of application of models
- Sustainable **software development in academia**. Normally, we get paid only for doing research, but NOT for maintaining software that can be of use in research
- Assemblies of materials, **cross sectorial phenomena** such as corrosion on dissimilar materials assembling....

- **Link between materials pre- and post-processing**. materials before being processed present many multiphysical challenges for modelling, while its influence in final structure's behaviour is more or less understood, but not the link between them.
- **Experimental data harvesting**
- Multi-scale sub-domain simulation systems : Zonal high resolution sub-domains for evolving material processes
- **Standardization** in materials modeling
- Models need to reproduce experimental behaviour and without experiments of recognized validity the rest are meaningless. Thus, the main effort should be devoted in collecting the highest level of quality in **experimental data**.
- **EDUCATION**: There should be action also in Marie-Curie, RiSe, etc. which considers early education as a crucial part of modelling and the digital future. This will garantee sustainibility since the young students will use the knowledge in their future jobs.
- Multi-scale modelling
- **applicability** and **availability** of the modelling and **transfer of know-how** to smaller producers, industrial designers, innovators, universities, associations, clusters, technology parks, accelerators
- The broad area of modelling all circular economy activities, combining industrial ecology **and life cycle management** principles, is missing. This topic is essential in creating sustainable products, i.e. products with minimum energy requirements and emissions in their life cycle. This is only possible with a combination of technological and societal competence in a broad holistically cross-diciplinary practice, avoiding reliance on narrow-minded reductionistic expertise. This reliance on purely reductionistic expertise is the cause of most technological failures of the past.
- **Changing the perception and culture in industry** towards simulation and its benefits of: saving time and money as well as promoting innovation.
- Self consistent scale jumping – **linking different length scales** in order to develop self consistent multi –length scale models
- **Topology optimization** cross-linked with materials modelling for structural application aiming weight savings while maintaining adequacy from strenght point of view
- continuum models
- environment and geopolitical aspect of strategic materials
- description of **transport across multiple scales**: apart from material properties, for applications/devices it is important to model electronic/phononic/photonic transport across multiple scales. The problems faced in these areas are similar to a certain extent, and can benefit and give inputs from/to material multiscale modeling.
- Multi-Scale-Modelling
- One very broad but underestimated topic is the **incorporation of SMEs in the material modeling**. A typical SMEs has the following heavy problems when thinking whether it should give a chance to material modeling: a) very high non-academic prices for commercial software packages - mostly there is no grading of prices depending on the company size (only a huge jump from academic to commercial price); b) not enough qualified staff; c) no possibility to employ a sufficiently qualified staff for a relatively short period of time required to model some particular problem; d) fear to give away some valuable internal know-how. The first item could be addressed by persistently asking software owners whether they can at least consider a possibility to introduce the

corresponding grading of prices. Items (a) to (d) require the establishment of medium-size private (may be, non-profit) research institutions which would take over the modeling of particular problems for different SMEs (companies). Such centers should have to their disposal the basic software packages for material modeling and employ highly-educated staff which could work both as translators and modelers.

- Materials **characterization**, systematization and catergorization for databases, for future prediction modeling
- Materials **discovery**. To use theoretical methods and modelling to propose novel functional materials and motivate further experimental work. The benefits of such activity for final business value are probably long term (> 10-15 years), but a thoroughly designed road-map towards theoretical discovery of new materials might help to accelerate the implementation of future revolutionary materials. To this end, efforts on the development of new structural search engines, structure-properties descriptor analysis tools, and efficient workflow schemes are needed at this stage.
- **Cognitive computing for material discovery**. We have simulations and experiments able producing large amount of data we do not even use. Published data is underused. Cognitive computing has a tool to search and find important information within the web relevant to our study is the next challenge for computers. Computers should be program to perform tasks we are not very good at. The next generation of computers should provide additional functionalities, e.g. a cognitive assistants able to retrieve relevant information from complex unstructured data. Find important correlation and suggest new possibilities. This combined with the traditional simulation tools can provide useful breakthrough in the material modeling. Think about IBM Watson winning Jeopardy in US: the computer digested wikipedia pages and was able to answer complex questions that require some "thinking". The same applied to materials could help scientist to focus on important tasks because helped by a cognitive assistant that does the boring part of screening tons of data.
- Advanced empirics **- rational model validation**
- Introduce **motivation measures for young researchers** to contribute to this very critical interface
- A closer connection between **characterization a**nd modeling to verify the goodness of the models.
- Development of **innovative numerical method** for materials modelling
- **Non-mechanistic modeling approaches** for nano-bio interactions. Given the lack of mechanistic knowledge regarding the interaction of nanomaterials with biological entities, it is fundamental to explore the development of data-driven models that will contribute to the discovery of mechanisms (i.e., paving the way to more general mechanistic models) and will facilitate the development of nanomedical applications and will also contribute to the impact and risk assessment of nanomaterials
- **Life cycle management** and recycling of new materials
- **Standards for calibrating model Parameters using experimental input**
- Extracting the **transferability** of different models (Note: transferability is different from accuracy above and more important. Uncertainty quantification etc. can only under certain circumstances predict transferability.)
- Ambient compatability and robustness of the materials
- data security and integrity
- **Systems Engineering** for Materials

- Computational Fluid Phase Thermodynamics
- Promotion of **education / training for the industry**
- **Deep learning** : How to lear from large database, and guess a new results with a high level of accuracy
- Controlling **dislocation/defects nucleation** during heteroepitaxial growth for optics/microelectronics is nowadays one of the limiting steps which hinders the development of highly efficient devices (such as Fin-FET transistors). The need to improve the modeling effort in this field does not seem to be adequately addressed.
- **Industrial application case studies**
- Extracting material models out of properties
- **Software**, **methodology**, model advanced development sustainability. **Benchmarking** and **reproducibility**. Credit.
- **topics that explicitly address ICME cases and translation scenarios**. Example: Enhanced batteries (Li-ion), energy conversion (thermoelectric), biodegradable high strength materials for compoentns etc. based on new technologies developed based on ICME and modelling.
- **Real demonstration** of modelling under operational manufacturing conditions
- Design of realistic and dynamic atom-scale models for description of interactions and binding of drugs/ligands with their membrane receptors. This topic is of extreme importance for the **pharmacological** field for the design of efficient lead drugs. There is reason to keep in mind that close to 50% of all proteins are in cell membranes, and a major fraction of these proteins and membrane receptors whose function is to take care of cellular signaling. If the signaling is impaired, the typical outcome is cancer. Given this, the biotechnology/pharmacology industry spends billions of EUR every year for the design of drugs targeting membrane receptors, in particular G protein-coupled receptors. This highlights the need to develop accurate models in a realistic setting, and the emerging impact of this development work that is crucial to the field.
- **Decision support** systems for integrating materials modeling into business processes
- Reducing variance in a chemical product. Improving analysis why the variance is taking place. Exact measuring.
- **Coupling** QM and mesoscopic
- **Materials Data Sciences and Informatics** is an overarching field of study that includes many of the components described above. This includes data, code, and knowledge databases, as well as e-collaboration platforms.
- The composites (both metallic or plastic based) are the future of the materials because they are the only materials able to overtake the limit of the ratio [weight/elastic modulus] imposed by the Nature in the common materials.
- Magnetic nanomaterials for energy, health and enviromental applications.
- **link from atomistic to continuum**; that would allow to create new materials or to assess the use of a specific material on an application basis
- Dielectric properties of soft condensed matter including the entire time/frequency scale from electronic polarization to restructuring in polymers.
- **Automated simulation workflows for the industry** - Maybe it's already included in topic #8, but here I'm thinking specifically to "turn-key" solutions where an industry can easily compute/obtain a given property of interest by inserting just system parameters. All the logic (sequence of calculations, bridging between scales, running on supercomputers,

numerical parameters, optimiztions) is taken care by the workflows, developed by experts in the field.

- **Adaptivity** of multiscale models
- Stimulate the research in developing new tools.
- Improved multi-disciplinary approach
- Virtual Multiscale Modelling: I think that connecting materials scale models and exchanging their data via the internet could give a boost to the modelling developments and will enhance the modelling performance enormously. I think that this is the major challenge for the coming years. Bringing models together, make them interoperable will create a EU-wide or global approach on modelling.
- Linked to topic 5, the need to **integrate material models with the processing** to converge more rapidly to new materials that have interesting properties but are also possible to manufacture at a realistic cost...As far as I can tell, processing and materials models are often not coupled.
- Open source versus licensed software. In many different areas a number of commercial codes are being developed, in competition with open source codes. An honest discussion on this topic (especially concerning the **sustainability of open source codes** and platform) would be beneficial.
- Multiscale modelling of nanoreinforced elastomeric Materials in order to be able to work under extreme conditions.
- **Software Engineering for Computational Science** --- some of the issues touch on above relate strongly to the way computational codes are developed: we need **tests to foster confidence in codes**, we need good documentation to make them accessible, we need to have good user interfaces (can be scripted or text file based) to make the tools effective, we need **computational workflow tools** to make sure input and output data are associated, can be varied and explored easily. The Jupyter notebook is a great workflow tool (see OpenDreamKit project) that will help with the last item.
- Development research and innovation actions that connect developers of different novel materials (polymeric, carbonaceous, metalic, nanoparticles,...) that can be integrated in new applications were their application is still limited. For environmental applications, further analysis and modelling about degradation and release of novel materials into nature must be analyzed for their social acceptance. In addition, the interaction of novel materials with existing systems should be also studied for a rapid acceptance in existing industries.
- Timescales/**configuration spaces** - the biggest challenge of materials is not size but **complexity** - only now are methods emerging that begin to address this problem and this is probably the biggest hurdle to widespread use of modelling methods by industry.
- Focus on scientific content and use excisting media for OPEN and FREE communication (in a way that everone can understand) rather than on administration and networking.
- Biomaterials/Biomechanics Modelling
- **Data-driven simulations** for material modelling and model selection, towards digital twinning of material systems
- In an area of fast expanding research a system of continuous **education** of R & D employs can help.
- Yes, as stated in our comments in Section(3), you do not mention **testing of materials** for input into FE analysis as a category. We feel this is a critical omission.

- **Testing materials** for developing models In order to model something you need to make observation of the material behaviour and furthermore a model must be validated by its ability to predict the behaviour in a situation away from the dataset giving rise to the model.
- Applications: I propose replacing/**complementing the "Manufacturers" working group by an "Applications" working group**. Their mission would be to gather information on "How can model X contribute to the application Y". If I was an industry member, that is not yet a fan of modelling, I would have never joined the EMMC. I would only be interested to join if I see that I can design better materials/processes for my application. This would also help streamlining the other efforts of EMMC since it shows what models can be used for what application, hence allows ranking of models according to their current and potential impact.
- **Inverse design**. Imagine you want a material with a property or function and you model backward to arrive at the atoms that are needed to produce that material.
- I am not sure how to formulate this briefly. More and more, non-experts are applying commercial software tools to model materials. Without the proper **education, expertise and experience**, huge mistakes can be made. The consequences of these errors may high significant impact. We could follow two routes: (1) make it very clear that these software tools are only to be used by expert users. This will not work. But: making it clear that materials modeling is a field on its own, might work. For that, we need clear 'good' and 'bad' examples; (2) accept that 'everybody' will apply the tools but provide **error estimates** as part of the result instead of relying on the user to be critical and responsible. In the end, I think we should pursue a combined approach. The reason why I believe that this topic is very important: at the moment that a lot of 'wrong' results are produced by non-expert users, the trust of companies in materials modeling will drastically reduce. We have to ensure that this trust should increase, instead of decrease, by having the right people working on the right topics with the right tools.
- **Improve interaction between academic world and industry** and expose student to the industrial modelling project in early stages of their curriculum
- Modelling of operational loads, and subsequent reliability and lifetime models (incl. load-dependent faillure models, probabilistic approaches etc.
- In my opinion we need to support community driven effort on **standardization** in ICME, allowing to organize workshops, discussion forums, etc. to keep this initiative going.
- Porting of codes and models on high end **HPC** systems
- Expansion of collection of published experimental information. The EU should be encouraging the **collection of experimental information** from far more sources. As it stands,much of this effort seems to have been around collecting molecular modelling data, but there is a very big need for **extraction and curation of experimental property meta-data**. Most efforts in this area have been limited by publishing practices and a lack of standard methods, but previous efforts in the pharmaceutical industry have shown the value of such methods (e.g. the ZINC database). We need an analagous type of effort for materials properties.
- Non-local continuum models including **peridynamics**. Non-local models are very important and they have the capability of functioning at mutliple scales by preserving continuum assumption.
- confidence and completeness in the material models. Avoid the valley of death: everything published in science but still **not sufficiently robust for industrial application**

- Development of physically based material relationships to be used in large-scale FE simulations.
- Design-enabling Modeling of Extreme-Scale Electromagnetic Interactions: i) insert quantum effects in the concept of electromagnetic (EM) systems, bringing established EM concepts and architectures at nanoscale levels; ii) control and reconfigure EM systems based on nano-architectures by nanoscale wave-matter interactions. This will enable the design of novel materials at different length scales at which elementary particles/quasi-particles such as photons, electrons, phonons and atoms “communicate”, interacting through mutual energy transfer.
- **Physically based reduced order material modelling**. Computer power increases steadily. However, the demand for computer performance are rising even faster, since new very promissing areas of material modelling (e.g. multiscale methods from atomistic to continuum, liefetime modelling) arise, which require enourmous computer power. Therefore reduced order models are important.
- support the use of predictive atomistic modeling in the design of novel materials
- **Validation** of material modeling: define and set-up specific experiments
- **Validation** of the models by experimental work using advanced characterization techniques
- **Optimization of the computation software** and methods to maximal effectiveness of using newly developed computer resources.
- In addition to networking activities and joint platforms for accumulating different communities and people also corresponding developments and agreements on **terminology** as well as common grounds for ways of collaboration are highly needed ! This can be done by raising curiosity ...
- Database for materials are limited to theory data. These are fragmented but with effort data can be joined. However, experimental data are hard to collect and they are mostly documented in literature (when not proprietary). Scavenging published data is a top priority. Some effort already on-going in the crystallography and thermo-chemistry community, but examples remain limited. Without **experimental data** it is difficult to use model data in an efficient and predictive way.
- Integrated simulation frameworks for physical\mathematical evolution of material : Smart automated multi-scale windowing for fast evolving material zones during processes
- Discrete-Continuum space and temporal **coupling**
- Addressing the issue of **high costs associated with software licencing** needed for material modelling.
- **Science of Complexity** – integration of novel deployment **in game theory** into mesoscopic and atomistic models in order to build multi –level models able to link consumer preference and market strategy, with consumer context experience and product formulation and processing
- **Better inclusion of the mathematical community**: multiscale models in mathematics are established, with their own nomenclature. It may be useful to involve more the mathematical community in the emmc, to benefit from already developed mathematical/abstract approaches, and to better establish the mathematical features and categorization of different models and couplings from a theoretical point of view.
- Ranked list of problems in the order of priority for modellers to tackle
- **Manufacture and service performance driven materials modelling**

- **Algorithms for massively-parallel and heterogenous compute platforms** (Computing is moving towards heterogenous parallelism. The computational challenges are enormous and will require massive amount of manpower to port existing codes to these platforms. Smart strategies (e.g. metaprogramming) are needed to partially automate this move.)
- Development of **hybrid** discrete (particle based) and continuum (field based or FEM) models. This models have recently shown their abilty to have a molecular (or even atomistic) representation but their computational efficiency allowed to bring them to large length and timescales.
- **Validation** of simulations against "gold standard" test cases and **validation** against industry set challenges
- **Innovation management**
- Setting a **norm** (like ISO) to ensure the quality and the trustfulness of calculations
- Connecting structure to function
- Another important topic is the modelling of the additive manufacturing processes, which is the future of the manufacturing.
- Inverse method for **multiscale** models
- Technology transfer between disciplines
- **Multiscale** modelling of Materials able to work under high thermal fatigue and creep corrosion strength
- **Open Science and Reproducibility** -- a lot has been achieved in terms of open source software, we need to push further to allow industry to trust codes their use. We should also work on making scientific results more reproducibly (by publishing codes, configuration files and computing environments with any results).
- Model **error quantification**
- Bringing together supply and demand by linking industrial need , sme's support and academia. An example would be the introduction of web based seminars along with web based **Brokerage** meetings since most of the community is expected to be e-friendly.
- **Testing materials for simulations**. When you have developed a model, you need data for specific materials. A flow simulation of e.g. injection moulding would require accurate date like viscosity, heat capacity, heat conductivity all complex functions of time, deformation rate, temperature and pressure. PVT data, mechanical date as function of structural orientation and temperature to simulate for example warpage. Each polymer is in principle unique, and generation of a full dataset will easily cost above 100.000 Euro. There is a need for an advance in not only simpler models but also testing to generate accurate data. Put garbage into a model and what you predict is garbage.
- New, **fast numerical algorithms** and procedures in multi-domain, multi-physics material modelling, enabling wide application of materials design loops on affordable computer hardware
- **standardizations** of models and data
- better **documentation** about the potential, limitation and parameter generation for material models
- **Characterization** of materials to provide reliable input data to models
- Connect and learn also more with **other modelling communities**, e.g. the protein folding and analysis of the bio-chemical community, especially in the case of (bio-)polymers where the overlap is very large
- Large scale **data post-processing**

- Evaluate model **efficiency** - how far outside its assumptions does a model still work well?
- Include **mathematicians** in projects. The capabilities of Industrial Mathematics seems underestimated.
- **Multiscale** modelling of selfhealing Materials
- European **repositories** of models
- highly skilled **mathematics** and informatics to capture the necessary physico-(bio-)chemical effects and corresponding models, e.g. via machine learning, artificial intelligence, chaos and fractal theory, parallel-, super- and possibly quantum computing, code optimisation, etc.

Section C: Complementary data

The primary field of application is shown in Chart 1.

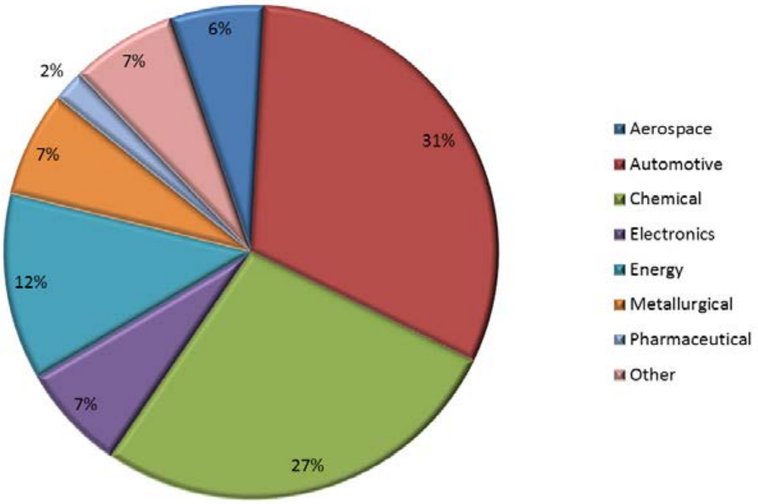


Chart 1. Primary field of application.

Automotive (31%) and chemical (27%) applications combined represent more than half of the total, followed by energy (12%), metallurgical (7%) with aerospace representing 6%.

Within the automotive applications, the dominant secondary application is metallurgical (36%), followed by chemical applications (29%). Within the primary chemical applications, energy represents 24% followed by metallurgy (12%) and electronic applications (10%).

Other applications mentioned in the survey include composites, polymers, fuel cells, coatings, optical coatings, photovoltaics, formulations, detergents, complex fluids, nano and microfluidics, memory devices, magnetic data storage, spintronics, organic electronics, adsorption engineering for environmental applications, water (environment), medical engineering, cosmetics, consumer care, construction, radiation protection, packaging, pulp and paper.

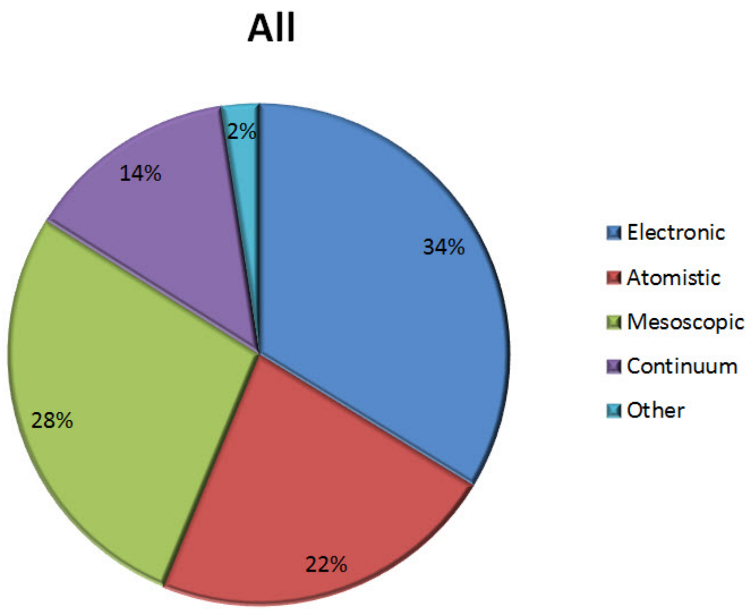


Chart 2. Models used in all application areas by all users of the survey.

Considering all entries of the survey, the dominant models used across all application areas are electronic (34%) followed mesoscopic (28%) and atomistic (22%). Among the contributors to this survey, 14% used predominantly continuum models.

User focusing primarily on electronic models (*i.e.* quantum mechanical methods) employ atomistic models as secondary tool and to a much lesser extent mesoscopic and continuum models. Users applying primarily atomistic models rely mostly on mesoscopic and continuum models as additional tools.

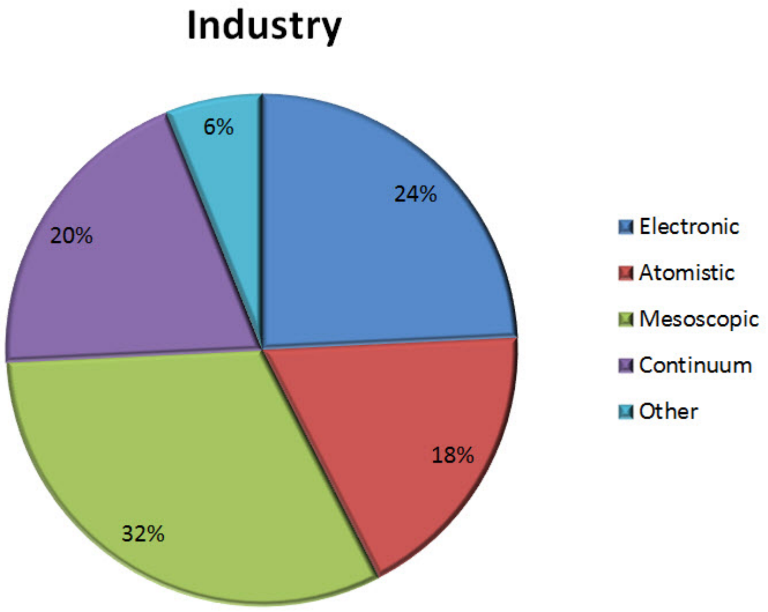


Chart 3. Models used in all application areas by all industrial users of the survey.

Considering only industrial users, the largest application is mesoscopic (32%), followed by electronic (24%), continuum (20%) and atomistic (18%). In other words, industrial users exhibit a stronger emphasis on mesoscopic and continuum models when compared with the entire set of users of the survey. This means that academic researcher employ more electronic structure methods and less mesoscopic and continue models. However, overall the distribution between e/a/m/c among the industrial users is not dramatically different from the entire group.

Concerning the use of multi-scale and multi-physics models, 57% of the participants in the survey provided a positive answer. This includes the separate use of, for example, electronic structure calculations and classical molecular dynamics simulations as well as the combined use of different models. From the survey it is obvious that there is significant interest in the linking and coupling of e/a/m/c. Comments made by the participants indicate that this is an active research area. In this context, specific codes are mentioned including OpenFOAM, COMSOL, LS-DYNA, COSMO-RS and MATLAB.