European Commission

Materials Modelling: Where do we want to go?

Research and Innovation

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Materials Modelling: Where do we want to go?

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INTRODUCTION

H2020 started on 1st January 2014 and in its second pillar, "Industrial Leadership", the programme LEIT (Leadership in Enabling and Industrial Technologies) focuses, amongst other areas, on advanced materials and nanotechnology. In order to kick-start the development of a **Policy for Advanced Materials and Nanotechnology (AM&N) Modelling, Simulation and Design** a one day meeting was held on 27th February 2014 in Covent Garden, Brussels, BE to exchange points of view among a range of stakeholders from the EU's materials modelling community.

A wide invitation was sent out to (250) experts to express their opinions on future needs for materials modelling, simulation and design. Participants submitted their input in the form of a focused presentation document, from which a number were selected to present at the meeting. The input can be categorized into scientific issues (extensions to the functionality of models) and policy issues (underpinning exploitation and commercialisation).

Extensive input on the state of the art in the materials modelling field was received. This input identifies the most promising areas for future research and innovation based on expanding materials models and is represented in the second part of this report.

During the meeting, the discussion was focused on necessary EU support activities (such as constituency building, research road mapping, market surveys etc.). The first part of the report presents the outcome of these discussions.

State of the art of AM&N modelling, simulation and design

Computational materials science has progressed into a predictive tool allowing explanation of the properties and behaviour of materials. Materials models fall into four categories: electronic, atomistic, mesoscopic and continuum models. The ability to integrate and communicate between these model types is a key factor for the prediction of materials properties and behaviour in operation. Experimental and computational data are needed to validate codes, to data-mine for high throughput approaches, and for model development.

The materials modelling community consists of many subgroups (scientists/engineers, electronic/atomistic/mesoscopic/continuum, physics/chemistry, hard/soft materials, open/closed source, etc.). Each application domain (energy, chemistry, transport etc.) has its own problems to be solved, but often show many commonalities at small scales. Materials modelling is also connected to High Performance Computing and Manufacturing and Engineering (mostly process and structural mechanics engineers using the materials models). In order to realise new materials often a new manufacturing process has to be designed.

With the recent growth in available computational power predictive multi-scale materials modelling has the potential to enable economic advantages for all manufacturing industries.

While computational modelling can transform the way we understand, and ultimately design and manufacture materials, some of these models have yet to become pervasive in industry. The lack of Research Road Maps on Materials Modelling is identified as a key shortcoming in the area. Market studies are also lacking, probably due to the fact that economic impact is indirect and hard to quantify; some software owners do not even have an overview of potential clients!

Most importantly, there is no organised modelling community that could represent all stakeholders. Cooperation (e.g. in the form of associations, cluster of projects, CSAs, infrastructure projects such as in the US) is largely missing today.

The EU can claim global leadership in modelling (especially in electronic and atomistic modelling and also in phase-field models and thermodynamics). However, this can only be exploited if complete materials model systems are created and when these are complemented by highly skilled actors who translate industrial problems into cases to be simulated with materials models.

Input received

In advance of the meeting, 88 input documents were submitted by the participants (some different inputs were sent by the same person or not worked out to full presentations). The presentations were categorised as belonging to three groups of stakeholders:

MAN: manufacturing and engineering industries ("the end-users").

SWO: commercial software owners (who sell materials models to end-users).

MOD: materials modellers (academic and industrial model developers).

The group of SWO consists of commercial and academic owners, but for both the software is available to third parties. The division between software vendors and software service providers was not yet made. Later it was realised that the software owned falls into two groups: continuum software owners who are not yet using any materials design software and materials design software (discrete and continuum).

Of these, 11 were presented orally to kick-start the discussion on policy support issues.
Written input was also provided by individuals who did not attend (9).

Note: While analysis of the submissions made provides useful pointers as far as priorities for policy directions and scientific and technical needs, it should be recognised that this is based on just 88 responses submitted by the 250 stakeholders invited to engage in the process. A future research road mapping exercise could provide the opportunity for a more statistically robust analysis of needs among the EU's modelling community.

The numbers of submissions made prior to the meeting were:

7 from MAN: manufacturing and engineering industries ("the end-users").

16 from SWO: commercial software owners (who sell materials models to end-users).

47 from MOD: materials modellers (academic and industrial model developers).

Input received – Policy

The most common themes that were raised in terms of future policy direction have been identified. A number of key themes emerged:

Key Theme	Relevant issues to be addressed and developed
Industrialisation of codes	User friendliness “Plug and Play” modelling by combination of codes Exploitation of modelling investments
Service provision	Required for SMEs without modellers
Creation of new actors: Translators	Analysis of industrial problems and translation in to materials modelling cases that can be simulated
Research Road Mapping	International survey of available models and codes Assessment of state of the art Extended International Survey to collect information on needs from manufacturing companies Prioritisation of material modelling needs Future strategy: development of new models
Development of modelling community and networking	For sharing methods, best practice, public engagement, training Encouraging the collaboration between modellers, software developers and industrial end users Clustered projects Establish communication and cooperation links between industry, research and academia
Integration of models and codes	Integration of different type of models and over multiple scales
Reliability and Quality; Benchmarking	Development of a chain of models with which realistic (=reliable, robust) simulations can be done. Confidence building via test cases where derived entities from simulation compare well to experimental measurements.
Standardisation	Standards for data/information exchange between models (input-output) European material database to share basic and advanced material properties data Terminology and syntax to express and represent the specific application (materials/component/device) simulated with materials models (approximated equations describing the behaviour of the entities)
Validation and references	Experimental materials databases Big data - informatics and data mining References to test suites and user documentation
Support from High Performance Computing facilities and activities	Required for truly multi-scale models and fast prediction, reproductability
Communicating with and educating the market (end users)	Case studies/Show cases/ Demonstrators showing models can be helpful solutions for practical problems. Communicate the benefits of simulation to industry (incl to SMEs) Incubators to gain simulation experience Develop new types of licensing schemes Cloud-Computing for use by SMEs

Table 1. Key policy themes arising from the meeting

Research Road Mapping

It was confirmed that here is a need for materials modelling research road mapping (state of the art, market survey, identification of bottlenecks, future research, stakeholders, etc.), focusing on electronic, atomistic and mesoscopic models and continuum models for microstructure evolution that can be used either self-standing or integrated in production processes in industry (linked to continuum models at the component scale). Such research road maps do not yet exist for the EU.

Exploitation of materials and nanotechnology models: Translators, the interface between Software Owner and End User

Consultancy/open innovation is not enough to propagate modeling throughout the EU's manufacturing industry. Experimental "end-users" have a lack of expertise that prevents them from fully integrating the tools into their workflow. There is a need for new players who have the ability to 'translate' industrial problems into cases to be simulated. These players could translate material models into methodology/workflows.

This function could, for example, be taken on by SME spin-offs commercialising material models and this could be supported by the EC SME programmes (feasibility studies, business plans). Also, training activities could and should play a role. A "hub" for placing industrial modelling questions and for providing benchmarking was an idea supported by many participants. This will allow the "democratisation of modelling" and allow the non-expert use of materials models that exist today, but that are not yet widely used by industry at large.

Exploitation can be supported by showing their capabilities to contribute to solutions of practical problems and to this end case studies, show cases and demonstrators should be created.

Organisation & structure to be considered: Council for Materials Modelling

The materials modelling community consists of many subgroups (scientists/engineers, electronic/atomistic/mesoscopic/continuum, physics/chemistry, hard/soft materials, open/closed source etc.). Each application domain (energy, chemistry, transport etc.) has its own problems to be solved. Materials modelling is situated in between, and is highly linked to, High Performance Computing and Manufacturing (mostly process engineers and structural mechanics).

A key recommendation is to establish a Materials Modelling Leadership Council that links all these communities. The Materials Modelling Leadership Council should build on existing communities that are structured around (types of) materials models and groups that deal with standardisation and validation. The Council should take advantage of the know-how and self-organization of the modelling community. Its function maybe guided by the following considerations:

- *Objectives:*
  - Exploitation of existing materials models:
    - Capitalise on existing knowledge in different sub-communities.
    - Ensure quality of simulation results.
    - Streamline interfaces between software owners and manufacturers.
  - Wide stakeholder management (industrial partners & software owners, key materials institutions):
    - Get software owning and end-user SMEs on board.
  - Provide inputs for EC future vision/plans:
    - Short and long term strategy establishment.
    - Research road mapping, identifying new needs/opportunities.
  - Promote and highlight model development (*targeted towards* industrial needs) done to obtain industrial trust in simulations.
- *Milestones:*
  - Adoption of material models (electronic, atomistic, mesoscopic) by:
    - Major software vendors.

        - Industrial end-users.
- *Performance Indicators:*
    - Year 1: Establishment of the council, research road map for exploitation of existing software.
    - Year 2: Establishment of translator players.
    - Year 3: Adoption of materials models by software vendors and industrial end-users.
- *Actors, Interests and Roles (ecosystem)*
    - End-users:
        - SME end-users.
        - Large industrial end-users (application-wise grouped).
        - Continuum software vendors including materials models in their software.
    - Translators (of industrial problems into simulation cases):
        - Modelling service providers.
    - Software owners
        - SME-owned software.
        - Large vendor owned software.
        - Academically owned software.
    - Material modellers (academics and industrial):
        - Electronic, atomistic, mesoscopic, continuum.
- *Activities of the Council*
    - Software Industrial Exploitation:
        - Hub (platform) for placing industrial questions and needs.
        - Establish translation service industry-materials (players, hub).
        - Ensure industrial quality (models, testing and benchmarking, advice on transferability across materials classes).
    - Supporting Measures:
        - Libraries of materials data and of materials models.
        - Database of industrial clients and simulation providers
        - Validation of simulation results.
        - Standardisation of links between models & experiments.
        - Research Road Mapping.
        - Inputs for EC future vision/plans.
        - Regulations: encourage the use of simulation to comply with regulations.
        - Interfacing to HPC.
    - Tailoring for industrial needs:
        - Per application area:
            - Benchmarking & Tests.
            - Show cases.
            - Training/Best Practice "Simulation Driven Product Development" Assessment.
            - Educating companies on best practices adopted by market leaders
        - SME end-users clustering:
            - Create incubators of simulation experience (autonomous entities with simulation experts and access to software and hardware for SME to get a cheap and risk free taste of the benefits brought by simulation).
            - Sponsor some large clouds with most popular software to be accessed primarily by SME.
- *Initial Volunteers for the Council*

Friis	Jesper	MOD	SINTEF	Norway	jesper.friis@sintef.no
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(Many others have shown interests to participate and all have been asked to present a work a plan and find the people who want to co-manage the activity.)

- *First Opportunities for Council Meeting*
  - Workshop on Validation of Computational Mechanics Models in Munich on June 12th, 2014 details at validmodels.wordpress.com.
  - ICMEg workshop from June 24th- 27th www.icmeg.info.
  - MSE meeting in Darmstadt in September www.mse-congress.de.
  - Italian Presidency event: Modelling Workshop 29 Sept till 1 Oct 2014 www.lets2014.eu.

- *International Cooperation*
  - The participants advised the EC that the following issues could be taken up for international Co-operation:
    - International database of material properties & processing data.
    - Libraries of models.
    - Curator quality stamps.
    - Exploitation of materials models/commercialisation.
    - Standardisation support to existing activities (KIM).
    - Efforts to improve models and workflows.

Input received: scientific and technical

The input received advised the EC on the needs for scientific and technical issues to be developed, and that could be the subject of future Calls under H2020. There was general agreement on the need to continue support for fundamental research, advanced software codes development and methodology development.

Participants at the meeting represented a wide range of communities:

- Authors, academic and industrial users of modelling and software providers of electronic, atomistic, mesoscopic and continuum methods.
- A variety of applications including additive manufacturing, bio-based materials, catalysis, ceramics, composites, formulations, metallurgy, materials for electronics and polymers.

There was broad agreement about the desire to **integrate AM&N modelling, simulation and design into the R&D process** and, in the longer term, to embed materials science models into business decision making. Such modelling and simulation-based Knowledge and Decision Support Systems would be an important step towards the following **long term goals** expressed by the participants (see Table 2):

- Ability to simulate materials and their emerging properties along the product process chain.
- Experiment, simulation and theory are fully integrated components in applied research.

- Materials options become an integral part of manufacturing and design decisions.
- Integration of real time modelling with real time process control.
- Translate customer/consumer requirements into materials design and manufacturing choices (reverse engineering).
- Prediction and control of materials ageing and in-life/service performance.

Vision topics

Table 2. Long term goals expressed by the participants

Topic	MAN	SWO	MOD
Simulation along the production process chain and materials options integrated with manufacturing and design options	x	x	x
Modelling as a component in applied research, same level as experiment: connect theory, experimental data and simulations	x		x
Ability to transfer end product application requirements back into materials design, Ability to do reverse engineering	x		x
Integration of real time modelling with real time process control			x
Ability to handle in-service performance and ageing.			x
Regulatory: Virtual testing and modelling considered in norms and regulations		x	x

A number of common themes emerged from the submissions and the discussion of high level requirements to turn this vision into reality. These are categorised in Table 3, and include the need for further method and methodology development, in particular for complex materials and conditions relevant to real systems; turning these methods into robust, industrial standard codes; the availability of high quality input parameters and the ability to integrate models and methods as a result of standards, and a seamless access hardware resources.

Table 3. Key science and technical themes arising from the meeting.

Topic	MAN	SWO	MOD
Accurate, predictive and robust models, including complex materials at realistic conditions	x	x	x
Model parameters: available, accessible, including experimental input, parameter determination and benchmarks	x	x	x
Standards and standardisation of models, parameters, interfaces	x	x	x
Seamless hardware access	x	x	x
Industrial codes of recognised quality	x	x	x
Flexible and easy to use methods	x	x	x
Integration and Components for plug and play Integrated Computational Materials Engineering (ICME)		x	x
High-throughput discovery infrastructures		x	x
Validated methodology and workflows for industrial applications		x	
Extending the scope (physics/chemistry) of a single model			x

Further detailed input on these requirements, as well as recommended actions, emerged along the following lines:

- Model and code development.
- Methodology and workflows.
- Model input data.

- Validation, benchmarking and standards.
- Infrastructures (hardware, software, data).

The input and discussion on these topics is further elaborated below.

Model and code development

The aim is to create a predictive, reliable and robust set of models across the spectrum (electronic/atomistic/mesoscopic/continuum). Eventually, this will lead to an integrated multi-scale capability that is easy to use and, hence, accessible to non-experts.

In most cases there was agreement that a lot of the models and codes already exist in Europe, and there is an opportunity to describe a wider range of phenomena and technology areas with current models.

The requirements are therefore: (i) the identification of core technologies of high quality, in particular models with rigorous physics, i.e. avoiding uncontrolled assumptions, (ii) further development in order to handle complex materials (e.g. multicomponent, multiphase) and their processing, thereby providing the ability to simulate the "evolution of material properties" at a wide range of external conditions, up to extremes (pressure, temperature, humidity, friction, radiation pH etc.).

There are also other instances where Europe can take the lead. In particular, there is still a need for truly integrated and scalable multi-physics codes, in contrast to current technology which tends to have multi-physics phenomena bolted-on which may not be sufficiently detailed to tackle complex materials physics.
Models for properties along the service life cycle are also still largely lacking due to the typically very long time scale of relevant phenomena such as ageing and corrosion.

Participants put forwards many suggestions for the development of electronic, atomistic, mesoscopic and continuum models as well as multi-scale methods, and some more high-level examples are listed below, in no particular order:

- Electronic models:
    - Approximate but accurate and transferable electronic models for large systems.
    - Further work on a range of properties calculated from electronic models (transport, spectroscopy, interfaces, energy conversion).
    - Methods for strongly correlated electron systems, excited states to model technologically relevant materials such as photovoltaic systems currently beyond the scope of conventional QM approaches such as DFT.
- Atomistic models:
    - Extending the timescales accessible to atomistic simulations.
    - Tackling thermally activated processes and rare events.
    - Fast and efficient ways of sampling complex potential energy surfaces.
    - Extensions allow to treat multicomponent materials
    - Extensions to allow predictions at high temperatures
- Mesoscopic models:
    - Extend nanoparticle/grain based models with statistical fluctuations for nano and mesoscale modelling.
    - Deepen and expand the understanding of mesoscopic methods.
- Continuum models:
    - Description of locally varying materials properties in components: structure -> properties constitutive equations including microstructure evolution.
    - Truly integrated and scalable multi-physics codes (strong and weak coupling)
    - Close the gaps in the modelling chain

- Multi-scale topics focused around:
    - Materials specific method (consisting of a chain of models) development for industrial applications e.g. in polymers and metals.
    - Models and knowledge that connects simulation output at electronic/atomistic scales with engineering properties (e.g. transition states to reaction rates, spectra to colour).
    - Coupling of (typically two) models that describe phenomena at different scales happening in certain applications, e.g.:
        - Link structural integrity at the macro (full structure) level with micromechanical models.
        - Linking between mesoscopic and continuum models: transfer of structures and morphologies calculated with discrete mesoscopic models to continuum discretisations.
        - Use of data provided by electronic, atomistic and/or mesoscopic models in continuum models at the scale of the microstructure
        - integration of data provided by electronic, atomistic and/or mesoscopic models in thermodynamic models and databases.
        - Transfer of data from electronic and atomistic models to mesoscopic models "on-the-fly (strong coupling)"
    - Further development of model integration, e.g.:
        - Method to decide where to use a finer type model
        - Direct and reverse mapping.
        - Adaptive coarse graining models.
        - Methods to estimate robustness of simulation chains including error propagation and sensitivity analysis.

Industrial Software and Methodology/Workflow for industrial applications

In order to reach the high technology readiness levels required for industrial use, methods and academic codes need to be further developed into robust, high quality software accompanied by methodology/workflow for applications.

The models that are needed to construct this methodology are either available or being developed (see also the requirements previous section). However, additional support is needed at the European level in order to turn great science and academic models into industrial software and to develop a: simulation methodology which is useful for industrial R&D.

Requirements and proposed actions include:

Industrial software:

- Establishing best practice in code quality, robustness and efficiency.
- Industrialization of codes (Code re-writes, pilots, demonstrations, up scaling, spin-offs).

Methodology/workflow:

- Software frameworks and concepts that enable integration:
    - Focus on components and ontologies based approaches that enable re-use in different applications and ensure consistency.
- Integration of tools from different scales into commonly used environments.
- Development of methodology for industrial applications. Validated, domain specific workflows integrate new materials development with process and engineering. Models and insights from different scales are utilised as required.

These developments will be a key element in "plug-and-play" Integrated Computational Materials Science and Engineering (ICMSE), whether it is integration into easy to use packages, or customized simulation workflows to fit specific industrial processes.

Model input data

All models, except the most fundamental electronic models, rely on various input parameters, and delegates pointed strongly to the need for comprehensive, widely available, easily accessible, validated quality input data for models at different scales:

- In the field of electronic models, some of the faster methods (e.g. DFTB) require parameters. Also a database of magnetic parameters (spin Hamiltonian parameters) from electronic structure calculations would avoid the duplication of efforts.
- For atomistic models, a range of force fields and parameters exist, but there are still gaps and there is often a lack of validation. An action would be to create a database of curated force fields; and provide parameter assessment of transferability across materials classes. Interaction with the KIM initiative https://openkim.org/ was suggested.
- For mesoscopic models, there are very few parameter sets currently available. A suggested action is to create a database of curated mesoscale parameters including assessment of transferability across materials classes.
- For continuum models and, in general, methods for parameter identification and determination: parameter development and databases with high quality experimental benchmark data. A database of models and parameters with validated usage conditions (temperature, strain rate etc.) was identified as a useful development

A related point is the general need for improved model setup and pre-processing general, i.e. better/easier/more efficient starting models.

The need for databases and assuring their quality was a recurrent theme in the input.

Validation, benchmarking and standards

There was a wide agreement on the importance of establishing a system of testing and validation and to set standards for data and models. This will build confidence in the software and workflow methodology, as well as efficiency in their application and integration.

For models, this means validation across a wide range of applications and materials rather than just a few examples as done in many research projects. Suggested actions include:

- Round robin tests.
- Research platforms that generate high quality experimental data for validation.
- Parameter identification standardization of methods to provide experimental input & direct comparison between experiment and simulation.
- Standardized method linking and data exchange.
- Consideration of different models providing different degrees of accuracy (and computational effort) for different types of usage (e.g. for fast decision making versus detailed trouble shooting)
- Focus on Robustness, Sensitivity & Reliability analysis. Error estimators must be an integral part of models, methods and experimental initialization data. This in turn enables:
    - Fidelity-quantified simulations: degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.
    - Risk-quantified design: using uncertainty quantification for robust optimisation and quality-by-design.
- Development of pre- and post-processing tools based on standards to increase the efficiency and accelerate the design of new materials and systems.

Infrastructures (software, hardware, data)

The goal is enable barrier-free access to input data, modelling software and the necessary computational hardware to run the simulations. Also, users should be able to exploit data from previous simulations to reduce the computational cost of their studies.

Suggested actions include:

- Continued close interaction with high performance computing facilities.
- Interfacing to HPC programmes on optimisation of codes (e.g. cloud software which can access 'Cloud' hardware), database technology and tools allowing effective searching and data-mining of such repositories, post-processing, integrating big data techniques with large scale computing methods for enhanced design and robust optimization etc.
- Data repositories with material structures and properties (e.g. enumerated materials and simulated properties)
- Databases and libraries of geometries and sub-models.
- Creation of an open-source high-throughput materials model chain.

CONCLUSIONS

There exist an impressive amount of materials design models, while its industrial exploitation is lagging behind. The profile of the submissions made to the meeting by each stakeholder group highlights a general point that, in terms of both the people involved and the financial investments made in modelling, there is currently a greater concentration of materials modellers (MOD) than of end users (MAN) in the EU's materials modelling community. A key aim of the EU's LEIT innovation programme is to help to move this situation so that there is much greater take-up of materials modelling by Europe's manufacturing industry, either directly by users in the manufacturing sector itself or via translators.

To help achieve this, the EC should develop an Advanced Materials and Nanotechnology Modelling, Simulation and Design Policy with the aims to:

- Establish a Research Road Mapping activity for materials modelling (state of the art, market survey, future research, stakeholders, etc.) focusing on electronic, atomistic and mesoscopic models that can be used self-standing or integrated in production processes in industry (linked to continuum models).
- Build an association of all stakeholders.
- Fill the "translator" gap: new players who have the ability to 'translate' industrial problems into cases to be simulated and who build streamlined interfaces. The council should serve as a contact point for people seeking advice in materials models.
- Integrate (electronic, atomistic, mesoscopic) material models into continuum models and industrial workflows of software vendors and industrial end-users.
- Improve coordination between software owners and end-users of computer based design of materials and training on industrial best practice (methodologies) for end-users.
- Industrialise materials models (benchmarks, quality labels, demonstrations, spin-offs).
- Develop model content (extension of phenomena that can be described) and shorten the development process of materials-enabled products.
- Drive and guide advanced computing and use of existing European facilities (interface to DG CNECT e.g. PRACE, up-scaling activities to support industrialisation).
- Strongly improve education and training in the area of computational materials engineering

The impact of the AM&N Modelling, Simulation and Design Policy should be:

- Short term:
    - Enhanced communication between the main actors through the creation of a Materials Modelling Leadership Council.
    - Channelling upcoming policy needs from the community to the policy makers.
- Medium term:
    - Creation of seamless model supply chain from the modeller to the industrial end-user in selected pilot areas.
    - Raising the awareness for such an approach as good practice in other areas where materials modelling has a role
- Long term:
    - Improved control of materials production and an improved control of concerned industrial products and processes.
    - Rapid deployment of advanced materials through predictive design of novel materials resulting in lower costs, lower environmental impact, reduced risk of product failure and increased product life time.

ANNEX: STATISTICS

The frequency with which each of the key themes identified in Table 1 was mentioned among the submissions is shown in the figure below. Here, the percentage of the submissions where the theme was identified is given for each stakeholder group (to provide a common baseline given the significant difference in numbers of submissions received).

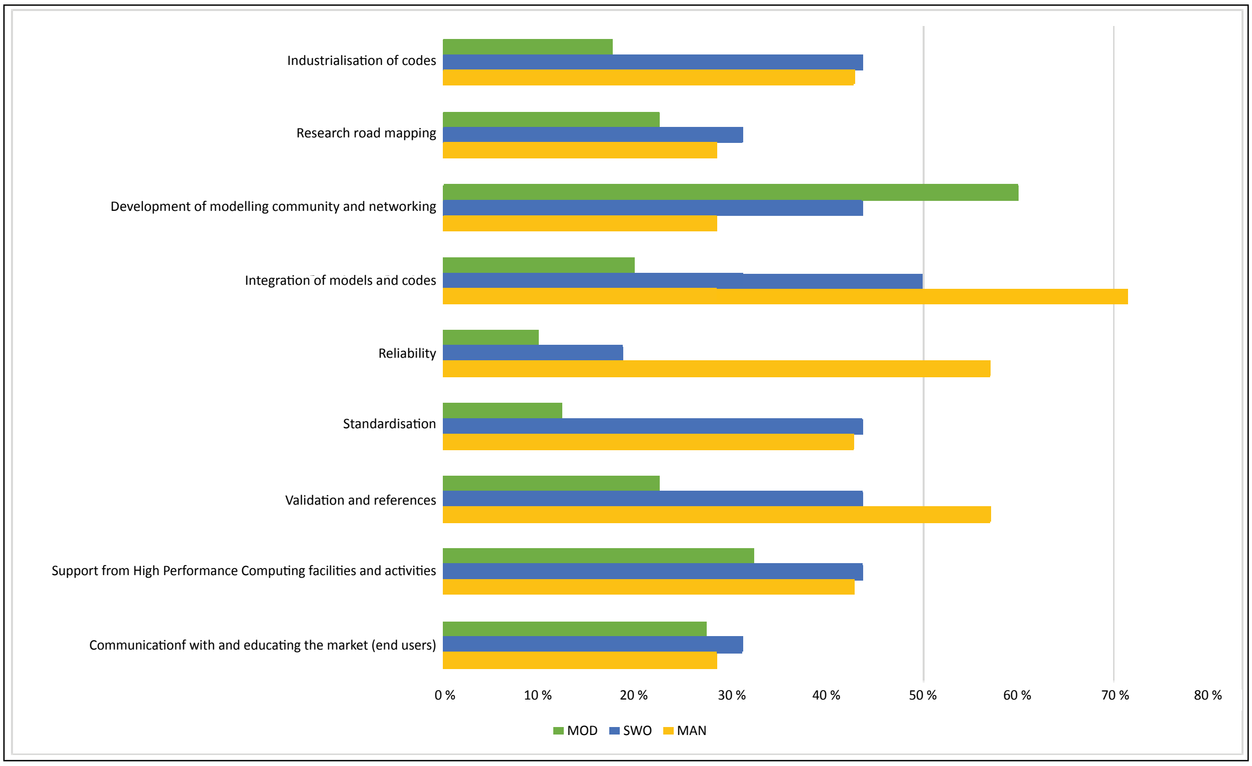

Figure 1. Percentage of submissions where each theme was identified for each stakeholder group

In the chart below, the percentage responses totalled over the three stakeholder groups is provided.

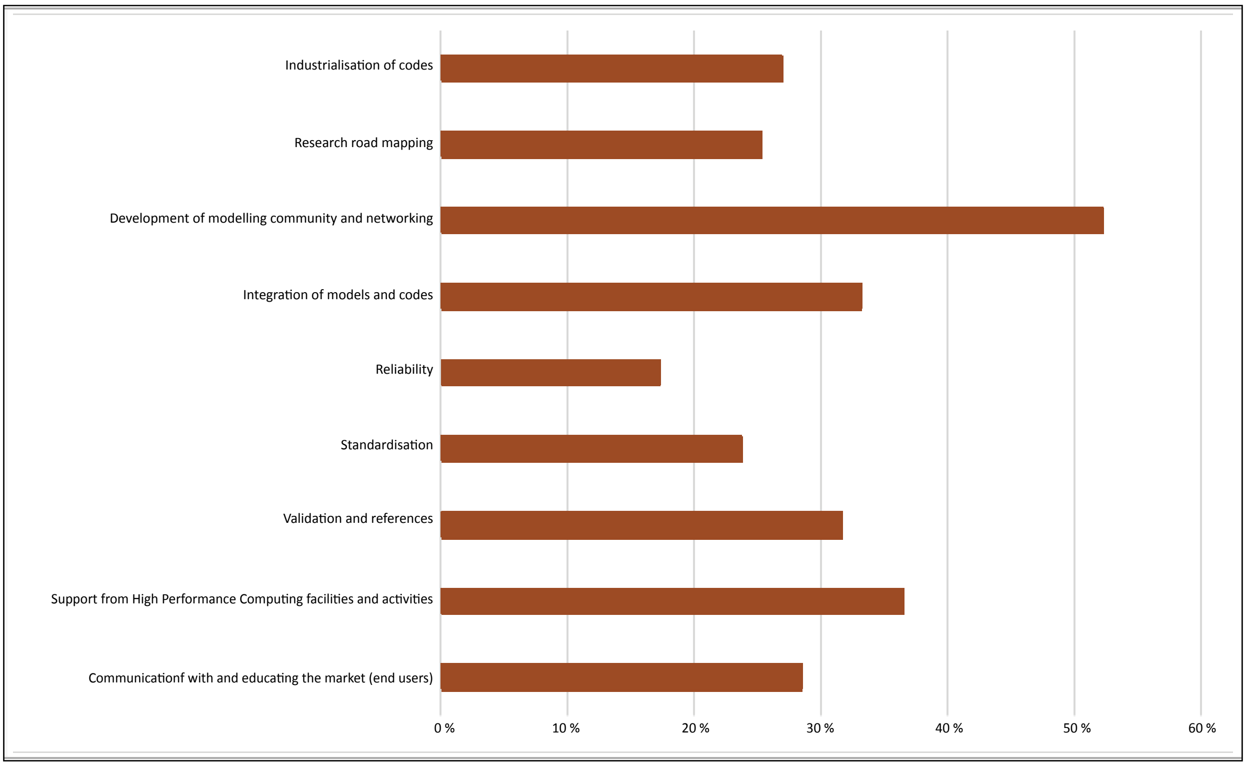

Figure 2. Percentage responses for each theme totalled over the three stakeholder groups.

A number of conclusions can be made from this analysis:

1. There is widespread support over all stakeholders for the development of an EU modelling community and associated networking. This is followed by provision of high performance computing facilities and the integration of models and codes.
2. There are quite large variances between the opinions of various stakeholder groups:
    a. For manufacturing industries ("the end-users") the top three key themes are:
        i. Integration of models and codes,
        ii. Reliability, and
        iii. Validation and references.
    b. For commercial software owners (who sell materials models to end-users) the key themes are:
        i. Integration of models and codes,
        ii. Industrialisation of codes,
        iii. Development of modelling community and networking,
        iv. Standardisation,
        v. Validation and references,
        vi. High performance computing facilities.
    c. For materials modellers (academic and industrial model developers) the top three key themes are:
        i. Development of modelling community and networking,
        ii. Calls for advanced code and model content development,
        iii. High performance computing facilities.

3. The greatest differences between the stakeholder groups are:
    a. End-users refer to the integration of models and codes much more frequently than modellers do.
    b. End-users refer to reliability as an issue much more frequently than modellers.
    c. Modellers requests calls for advanced code and model content development more frequently than either end-users or software owners.
4. There was relatively common agreement over the need for research road mapping and communicating with and educating the market (end users).

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The report is the result of a one-day consultation meeting held on 27th February 2014 in Brussels, Belgium. The consultation focused on necessary EU support activities such as constituency building, industrialisation of codes and research road mapping.
The objective of the publication is to raise awareness and to invite all interested parties to participate.

Exploitation is still lagging behind while manufacturers could speed up their product design, engineering and production with materials modelling. A newly created association of all stakeholders across sub-fields will have as objective to capitalise on past investments in AM&N modelling and will facilitate activities still missing in the field of materials modelling,

The target audience of this publication are manufacturing and engineering industries; process and design software houses wanting to integrate materials modelling; materials model software houses wanting to sell the software or wanting to provide services with the software and all materials scientists, who will undertake the necessary further development of the models themselves.

Studies and reports

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