Discussion notes

GENeral session: Interest of modellers

Scope of this session

Needs and requirements of industrial users (manufacturers, software owners and translators) will be gathered in the parallel sessions and will be presented at the parallel meeting.

In this session it is discussed what the interests of modellers are and how the global picture can be pulled together.

In a subsequent meeting in January the EMMC will consolidate a Road Map with industrial context and drive. And this discussion note is a first lay out for that Road Map.

Please state whether you agree with the following statements

I) EMMC Modeling Market Place Working Group

A steady and substantial progress has been achieved in recent decades in material modeling within Europe. Numerous modern numerical methods and software packages have been developed both by academic and industrial parties that, today, allow fast and reliable simulations of many material properties and systems thus allowing modeling of a large variety of technological processes.

The number of key players and stakeholders engaged in various modeling activities, including electronic, atomistic, mesoscopic and continuum (e/a/m/c) in Europe is rather huge. The explosion of the number of models (and the data related to models) makes it difficult to find the most relevant solutions in a timely manner and it is often unclear which models, and which software tools are available for a particular physics/chemistry problem. In addition models need to be linked to describe all relevant phenomena. This linking requires transferring of data and knowledge from one scale and model to another. Therefore demanding an efficient managing of data, including publishing, validating, linking, archiving and retrieving of modeling data and knowledge in a well-structured and standard form.

The modeling market place aspires to fill the overarching need for a platform that manages the materials data and knowledge infrastructure and provide an additional avenue for various EMMC working groups to achieve their goals. Such a platform will assist and further strengthen R&D foundations in Europe ensuring its continued leadership in advanced technology and modeling.

Needs and requirements on the MMP of industrial users (manufacturers, software owners and translators) will be gathered in the parallel sessions and will be presented at the parallel meeting.

The discussion should establish a first list of

- Actions needed to gather support of key representatives of industrial software owners, modellers, translators, educators and especially manufacturers and end users to discuss, prioritize and communicate the needs for a Modeling Market Place containing databases and librariers of models and data, validation and educational resources.
- Requirements for the design of a platform that leverages modern information technology paradigms allowing fast, efficient, secure and reliable information processing of the material modeling activities, knowledge databases and competences in Europe.
- Issues related to IP mangement and rule of conduct pertainning to openess of data and sharing

Please give your opinion on the following issues:

1. How to enable manufacturing companies (end-users) to do an effective search of numerical tools and/or providers of numerical simulations who could best suit their needs,

    a. How do we intend to achieve this? Here we have to ask companies what do they expect from an "effective search"?

    b. What are typical USE CASES?

    c. How to convince the end-users that this kind of search is useful and can be done without damaging the intellectual property of a company?

2. Supply software developers with comprehensive information about the potential clients and industrial tasks where numerical simulations would be highly desirable.

    a. How shall we obtain and collect the relevant information? - Here we will probably have to allow the companies to enter their need into an anonymous pool of 'simulation topics'

    b. How shall we present this information?

3. Ensure an effective information exchange within the academic simulation community to enable faster general progress of material modeling methods.

    a. The very first issue here will be - how to convince the academic community that they need additional information exchange channels (I mean, in addition to the existing ones like publications and topic conference)?

    b. What needs to be done in practice? New citation mechanism with faster turn around without breaking existing paradigms?

c. How should Data and model repositories be realized?

d. What needs to be done to reach such data and model repositories?

4. IP issues: we need to take into account public funding vs. proprietary research. Do we need other channels that allow “sponsored research”?

5. Setting standards and requirements of modeling data repositories including possibly data, modeling codes and validation repositories.

   a. What needs to be done to achieve this goal in the future? What is the best path to at least a *de-facto* standard for data (including experiments)?

   b. Why are standards important? (sustainability, efficiency, interoperability, boosting R&D, linking and coupling data)

6. What web technologies are available? Can we use current ones? Or do we need to design new ones?

7. How to collect the information needed for the database of actors, and how to make it public
8. Privacy issues as well as IP, rules of conduct and authenticity of information?
9. Who will be responsible for the data integrity? (open “social” platform)
10. How do we plan to reach a critical mass?
11. How do we plan to make this market model place sustainable?

II) Materials Model Capabilities

The development of new materials and their optimal use across industries is a significant innovation driver and a key factor for the success and sustainability of the industry and European society in general.

Large and small companies rely on numerical simulations to effectively and efficiently design and engineer new products, and thus minimize the need for prototyping and testing. While different industrial sectors have different target materials with a variety of modelling needs, numerical simulation in industry tends to be dominated by Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) solved by Finite Element or Finite Volume Methods, and forms part of the Product Lifecyle Management/Computer Aided Engineering (PLM/CAE). This simulation of manufacturing processes, devices and products started more than 50 years ago, is mature and served by a limited number of multi-billion dollars software companies.

The parameters in the SM or CFD models are usually determined by experiments. As a consequence, the influence of the materials' chemical properties and their macroscopic performance in the end-product are usually missed! More and more companies have recently started using electronic/atomistic/mesoscopic materials modelling to include more detail in their simulations to treat new effects, describe more complex systems, or aim for more reliable modelling results. This development is both promising and challenging. However, with the increasing importance of materials for the European competitiveness and sustainability, it is indeed urgent today to develop such more complex models, and the software tools that go along with them, and to let these models and tools mature for an effective and efficient use across various industry sectors and application areas. Here it is clearly important to also spread the information about such new developments and to promote (e.g. via training) the use and best practices of materials modelling in industry and for industrial benefit.

Needs and requirements on the model development and application of industrial users (manufacturers, software owners and translators) will be gathered in the parallel sessions and will be presented at the parallel meeting.

This document gathers the input from modellers who are developing novel models and/or designing novel interfaces to couple and link existing models. In a subsequent meeting in January the EMMC will consolidate a Road Map with industrial context and drive. And this discussion note is a first lay out for that Road Map.

The discussion should highlight some of the following aspects.

1) What are the most serious gaps in the industrial applicability of existing models (and the entailing software)? How do we go about identifying them? And how do we best fill them?

For the creation of an effective platform for communication and joint progress among different stake-holders it is crucial to increase the awareness among modellers of the industrial needs, and vice versa, to increase the end-users' awareness of the capabilities, both possibilities and limitations, of existing models and modelling techniques, as well as of the new possibilities that new developments can bring. The Software owners working group has began to identify some of the gaps in the industrial applicability of existing software. These limitations could implicate a need and potential for wider and shrewder exploitation of existing models, and. on the other hand, the development of novel or improved, more accurate (yet computationally feasible) models of industrial relevance. Some examples include novel models for electronic structure (both wave-function-based and DFT-based), reactive force fields for molecular dynamics and mesoscopic models with tuneable coarse-graining. An endorsement by the software owners working group is definitively essential for supporting other initiatives aiming to widen materials models.

2) What new schemes for the coupling/linking of models (existing or future) are the most needed to promote industrial applications? How do we go about identifying them?

For industrial problems, sometimes it is not yet well known how best to couple and link different models between, or within, the electronic/atomistic/mesoscopic/continuum chain in a satisfactory way. For example, in linking electronic- and atomistic-type models "upwards" for a certain material, it is usually not known which of the physical and chemical features of the electronic model that need to be carried over to the atomistic model to preserve the crucial elements of the description, nor what model expression is needed to capture these features. Going in the other direction, i.e. "downwards", is often even more problematic, with a range of possible approaches for reconstructing the missing information. Hence advanced physics-based coupling/linking models and interfaces are needed, which are targeted at materials and processes of industrial use. The most promising interfaces should be identified and they should receive an endorsement by the software owners working group.

3) How to receive endorsement from software owners and manufacturers working groups?

The EC LEIT Programme "Industrial Technologies" aims to help solve the problems felt by the wide European industrial constituency. If modellers want certain activities to be funded, they have to present that they meet a wide European industrial need and they have to receive an industrial endorsement. Hence a list of activities must be defined and then proposed to industrial members for endorsement.

4) How can one motivate modellers to make exploitable software?

In order to use academic software codes in industry the codes should be actively transferred to third parties via licenses.

Licensing considerations:

- Restrictive licences - Commercial/Proprietary. Protection of the source code (only complied software provided) and customer uses the software under a licence agreement that only allows them to use the software, not to sell it on. The customer does not 'own' the software, only a licence to use it. Licences may be periodic (e.g. monthly, annual) or perpetual and may come bundled with or without maintenance (upgrades, support etc.).

- Open Source Permissive licences – Generally free distribution with no limits on modification and licence changes acceptable if © notice retained. Similar to, but not exactly public domain software.
- Open Source Persistent licences –GNU Lesser General Public Licence permits certain programs, usually sub-routine libraries to be licensed under Free Software Foundation (FSF) license, but to link to non to link to non-GPL software.
- Open Source Persistent & Inheritable licences – GNU General Public Licence: free distribution, no limits on modification, all bundled and derivative works must be under GNU GPL.
- Dual licensing - simultaneous use of open source and proprietary licences – use of both open source and proprietary licences for one product.

In order for academically developed software to be employed by industry the software should be written according to certain standards. Wrappers should be available. Special attention should be given to integrate electronic, atomistic and mesoscopic models into continuum models. Documentation of the software code should accompany the software.

- Which licenses can meet the wishes of open source developers and proprietary software houses?
- Can code from the start be written for exploitation purposes?
- How can possibilities for service provision and maintenance and user training be incorporated from the start? Is there a need for training of physicists and chemists on software developing skills (scripting, automating and packaging (not usually in their expertise…)
- How can data and exchange standards be taken into account? Are the necessary wrappers developed? And the necessary homogenisation tools?

5) What is the most effective way to gather the key representatives of the academic modellers to discuss, prioritize and communicate the needs of materials modelling?

There is a strong need to develop an exhaustive survey of different modelling approaches within electronic, atomistic, mesoscopic and continuum categories, to understand the key underlying ideas and to highlight their advantages, limits and drawbacks. There is a need to recognize qualitatively similar ideas and modelling approaches, to identify overlaps, and to identify complementarities, in order to fully explore the potential and to get sufficient recognition.

6) What can the EMMC do on top of existing activities?

III) Open Simulation Platforms

Needs and requirements on the Open Simulation Platform of industrial users (manufacturers, software owners and translators) will be gathered in the parallel sessions and will be presented at the plenary meeting.

Continuum models in most cases provide the link between products and production processes and the materials constituting the components of a product. Continuum models need to be linked to discrete models to give accurate results. Coupling an linking numerous continuum models across all scales and along all process steps and bridging between discrete and continuum model worlds will require substantial effort with respect to harmonizing and standardization of information exchange, which can only meaningfully by a European or even global effort. Free availability of a respective platform infrastructure requires substantial public engagement at an international level.
Key 'market problems': Materials product design requires mastering "multi-physics" and "multi-scale" effects. Using current, monolithic tools to deal with each case is time consuming and expensive, not good enough for MAN! An attractive solution is to reuse existing tools: link/couple and integrate them and this approach has great potential to MAN, TRANS, SWO….

Harmonizing and standardization of information exchange needs

- ***Data and software interfaces* (API wrappers)**
- Data and exchange standards
- Necessary wrappers

and the EMMC should find ways to ensure these are used!

1. What are the needs and requirements of modellers for an Open Simulation Platform?

2a. How to reach a common standard should be discussed and this probably needs to be done in a dedicated EMMC Standards Working Group (SWG).
2b. Can a Plug & Play architecture be supported?

A first CORE of standards, focused on continuum (with elements from /e/a/m/) is under development in EU projects. The EMMC will build on to this existing work and targets to complement it as much more is needed.

Activities in the EMMC

- Scope is to have a limited number of platforms (covering wide range of scales and methods) being available in 2016.

  Note: First versions of some of EU project platforms are expected to be ready in 2015 along with initial specification drafts of working and implemented standards (data and interfaces) and can provide input for the core standard (2016)

- Establishment of the first core of the EMMC Standard Working Group (open to all)
- First draft of a harmonized standard based on the specifications published on www.emmc.info
  Note :the EU project ICMEg will in 2015 deliver a survey of modeling tools; identification of issues requiring standardization and deliver a drafting of a a standard based on the survey
- End of 2015: EMMC to combine the draft based on the survey with the early draft of the SWG
- Beginning of 2016: releasing second draft of the combined standards (on the web as above)

  Note: April 2016 second CMEg workshop on identification of missing issues on the basis of sandbox-scenarios and respective complementing the standards

  September 2016: Manuscript for book on standardization available
- End of 2016 – beginning of 2017(?): releasing third draft of standards by EMMC (on the web) and officially establishing an open Standards Working Group together with ICMEg

4. Can a meta-model be developed?

IV) Validation of materials models

Needs and requirements on the Validation of materials Models of industrial users (manufacturers, software owners and translators) will be gathered in the parallel sessions and will be presented at the parallel meeting.

Industry has established procedures for experiments to be conducted after DIN norms and certified procedures to qualify materials for end-user applications. E.g. the development of materials and their production equipment for safety relevant applications relies heavily on such procedures to ensure trust in the use of these materials. Industrial communities as aerospace are extremely careful to switch to new tools even if they could achieve faster and cheaper materials development processes.

The drawback is that such procedures are time consuming and carry great costs. Therefore, a 'cultural' transformation of engineering needs to be tackled to embrace simulation based materials design. To improve the acceptance of materials models and model systems, experiments can be utilised to evaluate and validate these models and establish a trusted process to incorporate more models into the materials design and manufacturing processes.

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

The discussion should highlight some of the following aspects.

1) How can the modellers contribute to this obvious need?

2) Identification of experimental techniques which can:

- provide validation for models under development:
  The continuous process to develop and enhance models to describe materials properties and behaviour needs a tight integration of specific experiments which can help validating the progress. The goal of this WG is to (help to) identify the necessary experiments on the time and size scale which the modellers need for validation. The goal is to make the process of modelling more efficient by being able to validate a stepwise development
- provide validation on the limits of accuracy of **single** models describing materials behaviour for a set of application relevant parameters (e.g. depending on temperature, stress, lifecycles, atmosphere, compostions):
  The goal is to define a database of certified models (link to electronic, atomistic, mesoscopic, continuum and Multiscale Models groups) which can be used to solve specific problems or can

be combined into model systems. Furthermore, the database for the experimental validation allows to estimate the error in the model prediction depending on the evaluated parameters.

- validate, ascertain and certificate **model systems** describing complete parts or systems such that they can directly and safely be used in process modelling and as a Business Decision Support System(link to the open simulation platform and Coupling & Linking and BDSS working group)
The goal is that the database on experimental techniques allows to certify model systems which contain several models linked or coupled together e.g. to describe complex parts. The link can be across time and length scales or combine different physical aspects of a material or it can combine models containing competing mechanisms describing transitions between different materials behaviour.
- integrate specific and novel experiments (e.g. high-throughput and combinatorial experiments) to bridge gaps between models (e.g. in case of linked and coupled models):
The goal is to identify together with the other WGs where experimental tools can or need to be integrated to link existing models into model systems in a seamless and fast way. The goal is also to make the transition easier for industry partners to integrate models and experiments into their materials design, optimization and validation processes. By identifying experiments which can bridge gaps, the goal is to make the process more robust and reliable and reduce the risk of investments. The integrated experiments can provide material properties and behaviour as input parameters for other models in situations (e.g. above a certain alloy content, above certain temperatures) where other mechanisms become active, which are not yet fully (fully) available through the models.
- provide a reliable database on experimentally measured materials properties and behaviour to support the benchmarking of advanced materials models:
The goal is to provide a growing open database containing certified materials properties and behaviour, and estimations on the error involved, across a clearly described parameter set, acquired with documented testing equipment. The data reliability shall be enhanced by the organization of Round Robin tests. The database should enable the comparison of materials properties and behaviour acquired by different techniques and connect the data to certified models and model systems.
- help identify mechanisms (e.g. deformation mechanisms) through novel in-situ experiments or analytical tools to complement available models:
The database should present experimental tools which can be used to identify physical mechanisms when the prediction of models is breaking down.
- establishing the outline of a data repository for citeable experimental output (e.g. raw data), experimental boundary conditions (e.g. machine, experimental parameters,…), experimental error, and links to experts and labs:
The database shall have an easy access, through a simple and easy to use but flexible user interface for input and output.
- educational test cases, showing how experimental data can be connected to simulations: specific experimental data from the database can be used to educate trainees on how experiments and simulation interface and how experimental data can be used to validate models and boundary conditions.
- To facilitate the use of the database procedures and help files shall be included. The database will also be linked to the model marketplace.