



Charter and Mission of the EMMC Modeling Market Place Working Group

Executive Summary

Modeling Market Place (MMP) is a platform for the information exchange on key issues concerning materials modeling and its industrial application and is focused on exploring possibilities of, and offering novel solutions based on information technology to the entire European material modeling community.

Background

In the recent decades, a steady and substantial progress has been achieved in Europe in the field of numerical simulations in general and in material modeling in particular. This allowed Europe to take a leading position in materials modeling. 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 (e.g. chemical, mechanical, thermal, electric and magnetic characteristics) and thus allowing modeling of a large variety of technological processes.

Traditionally, industry has relied on continuum models, solved with methods such as Finite Elements (FEM) techniques mostly for structural mechanics and Finite Volume Methods for Computational Fluid Dynamics (CFD). These models have been integrated in Product Lifecycle Management and Computer Aided Engineering (PLM/CAE) approaches. This extensive use can be attributed to the ability of these continuum models to provide a description of systems on device (i.e., product) relevant scales.

However, with the advancements in nanotechnology the shortcomings of these methods became apparent as they do not apply particularly well to small scale problems happening at nanoscale and beyond. A need for materials models for the materials development emerged. It is anticipated that the extension of the current PLM/CAE systems to include more details of materials would bring many new benefits.

The reliability and predictability power of product/device modeling can be augmented by integrating well-established models applicable to large scale areas with modeling methods that describe the system on smaller scales. Such an interlinking requires transferring of data from one scale and model to another, therefore demanding an efficient managing (publishing, archiving, retrieving, etc.) of modeling data (i.e., input and output, parameters used, validity tests, literature, etc.) in a well-structured and standard form.

While there are a limited number of well-established stakeholders offering models applicable to macroscopic scales, the number of key players and stakeholders engaged in electronic, atomistic and mesoscopic modeling in Europe is rather huge.



Managing data and models

There is no exact estimate of how much materials science and engineering modeling data exists, or of how much is currently produced in the many individual laboratories and companies around the world. There is a need to collect this data. Additionally, neither a standard for organizing modeling data nor the related information technology infrastructure for storing such data exists.

The explosion of the number of models (and the data related to models) makes it difficult to find the most relevant solutions, and it is often unclear which atomistic, electronic or mesoscopic models, and which software tools are available for a particular physics/chemistry etc., problem.

Collaboration and information exchange

Another important issue is that due to the rapid development of many novel modeling paradigms different subgroups of the 'simulation community' are often not sufficiently informed about the state of the art in the neighboring areas. This circumstance considerably hampers further progress of multiscale models.

Educational resources

Often the end-user wonders what user expert level is and the infrastructure necessary to use the models efficiently are unknown. Without knowing the risks and gains of model usage, industry does not want to make management decisions and invest into novel (integrated) ways of materials development.

Validation of data

There is a lack of systematic information regarding the validity, i.e., the limits of applicability of a particular method to a particular problem. No readily available information on the comparison of the modeling results with experiments exists, further hampering the adoption of novel modeling methods in industry. As a result, the industry in general and SMEs in particular remain largely unaware of the rapid progress of contemporary numerical modeling tools, so that this powerful possibility to predict the properties of new materials and to optimize technological processes 'in advance' is still strongly underutilized by the manufacturing companies (end-users).

Scope of the MMP WG

There is therefore an overarching need for a platform that manages the materials data infrastructure. Such a platform will assist and further strengthen R&D foundations in Europe ensuring its continued leadership in advanced technology and modeling. The scope of the material modeling market place is therefore to investigate and provide a design of a platform that leverages modern information technology paradigms allowing fast, efficient and reliable information processing of the material modeling activities and competences in Europe. To this end, the modeling market place will explore networking, computing systems software and associated information technologies to propose possible



solutions. The MMP aspires to offer coordination opportunities to extract knowledge and new information from large and complex data collections. Europe has the opportunity to tailor the platform to Europe's own needs.

The scope of the MMP is closely interlinked to those of numerous WG within the EMMC, in particular the Open Platforms, Translators, HPC, and Business Decision support WGs. The focus of the MMP is more on exploiting information technology, providing thus another channel or dimension for the efforts in other EMMC working groups.

General Objective

The primary objective of the Model Market Group team is to ensure the broad, fast, and easy information management and exchange both between the modeling community and industry and within the modeling community. The objective is to

- i. 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,
- ii. Supply software developers with comprehensive information about the potential clients and industrial tasks where numerical simulations would be highly desirable.
- iii. Ensure an effective information exchange within the academic simulation community to enable faster general progress of material modeling methods.
- iv. Setting standards and requirements of modeling data repositories including possibly data, modeling codes and validation repositories.

The creation of the corresponding 'informational environment' is crucial for a smooth and rapid transform of the contemporary scientific knowledge and modeling experience to the industrial clients (and thus to the society in general), because the insufficiency of information links between the areas of fundamental material modeling and their potential applicants (beneficiaries) represent at present one of the major obstacles for further progress of the material science.

Specific Goals

In order to achieve the general goal outlined above, the group aims to develop, offer to the community and maintain the following informational resources (most probably in form of websites with corresponding databases):

1. **General database of companies and persons involved in development and applications of numerical models** (Database of Actors)

This database should include the following five groups of users:



- Fundamental scientists working on the development of new numerical methods which can be potentially used for the development of new software for material modeling (MOD)
- Software developers who would like to offer their software and/or their services to industrial clients (SWO)
- Companies which are looking for (or are potentially capable to use) numerical modeling for the improvement of their products (MAN)
- Translators who provide research to industry based on materials modeling (TRANS)
- Companies who provide support to materials modeling in the form of measurements, characterization, visualization, HPC etc. (SUP)

- 2. Platform for modeling expertise exchange** The MMP users, representing, MOD, SWO, MAN, SERV, TRANS, SUP will be able to participate in an open list of board of experts in all materials modeling areas. The users can be queried by keywords and other semantic data and contain a brief, but understandable (also for a non-scientist) description of the area of competence and skills of these users and their offering. This board of modeling experts may be initially co-managed by MMP and other interested EMMC-WGs, such as the Translators, BDS, HPC, and Open platforms. We emphasize that this should be an open collaborative site, enabling users to get in touch with other experts fast, establish new collaborations, and also apply for paid service through the MMP or to seek or give advice and guidance.
- 3. The educational and training resource**
This platform should contain web-links and offer other useful materials (e.g., information about seminars and webinars) for persons who would like to make themselves familiar with specific numerical methods and/or to improve their skills
- 4. The resource with the list and description of open source and proprietary solutions**
In many areas of materials modelingⁱ there exist a variety of reasonably well developed freely available software codes that can be used for general modeling purposes. There are also many proprietary codes with industrial support and maintenance. This resource should include the brief description of these tools; abilities should be listed together with the links to the corresponding homepages. The resource should be also searchable by keywords (preferably hierarchically ordered). The MMP will focus on the IT that allows such a platform, where the content is expected to be provided by the EMMC SW owners WG
- 5. Benchmarking site**
One of the most difficult problems in modeling is the validation of results. For this reason we intend to provide a web resource, where we would like to collect the so called 'standard' problems, i.e. problems which can be used for comparing results of simulations for the same problems done with various software packages. In the ideal case the problem should be treated also experimentally in order to verify the relation of these simulation results to 'real life'.
- 6. Validation through experiments**
The site will also provide a list of experimental techniques which can provide benchmark data,



input parameters and allow the comparison to standardized validation measurements. The aim is also to provide insights into the reliability and errors associated with the experimental techniques, experimental alternatives and expert contacts to find the best possible partner.

Openness of the platform

The MMP will aspire to lay down the foundations for open science in the form of an open community forum. That is, there will be no gatekeepers, and thus no judges (Open collaboration platform). The aim will be to launch such a service first using existing web services (e.g., mediawiki or Joomla, Drupal, wordpress, etc) and help it in the beginning until it gains momentum. After that, it is on its own. However, it may be necessary to allow for a special service to be offered through the website on a paid basis for those companies who would like to get the service and use it without disclosing any information. Such a sponsored service will contribute to the future long lasting sustainability of the web service

Desired outcome:

The outcome of the MMP would be a document of general requirements for an interconnected suit of websites and databases with easy to use front ends allowing users (scientists, engineers, managers in industry companies, students and educators, etc.) to search and obtain reasonable information efficiently and in a timely manner. In addition this service will provide smart networking and modeling services. These web-services will be powered by powerful and novel information analytics systems in the back-end designed specifically for the needs, goals and requirements of the European advanced nanotechnology and materials engineering community.

Timeline:

- September 2014: Updating the Charter/mission and allowing new members to give feedback
- November 2014: organizing a session in the kick-off meeting, possibly in collaboration with other WGs, introducing the mediawiki capabilities and vision of the MMP. Interlinking with other WGs. Goal is to achieve awareness for the current services and initiate discussion for future collaboration and interlinking different working groups.
- Completion of the first version of the a web-service collect information to the database of actors by end of Q1 2015
- Completion of the design of the public website and incorporating automatic registration and reviewing of new applications by end of Q2 2015
- Q4 2014: First draft of USE CASE of the Database of Actors
- Q4 2014: First Draft of USE CASE of the Board of Expertise Exchange



- Q1 2015: review of the charter and update with further USE CASES and laying a roadmap for the composition of the general requirements

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ⁱ http://ec.europa.eu/research/industrial_technologies/pdf/modelling-brochure_en.pdf