



Discussion Note

Manufacturers group

Material Modelling: Industrial Needs and Specifications

Please state whether you agree with the following statements

Manufacturing companies across Europe (SME's and large corporations alike) recognise the potential of materials modelling to drive a radical change in speed of product design for and cost of manufacturability and in-use performance. Although applications to both material and manufacturing process design have been demonstrated, modelling is not always on the critical path of commercial development because modelling tools are often seen as too difficult in use, not accurate enough, or unable to get answers to very specific questions.

In a tough, highly volatile and competitive market environment, speed-to-market is critical, especially for companies that need to put differentiated products on the market every year. Materials modelling-led product innovation is a key differentiator for success in such competitive markets. However, there remain a number of technical challenges to develop predictive models that are easy in use and affordable yet accurate enough to enable the desired novel product design. Successfully addressing these challenges reduces the time to market and development costs of differentiated product offerings leading to major benefits and enhanced competitiveness for the European Industry base as a whole in a global economy.

The future of the European industry depends on a strong European-based materials modelling capacity; such leadership can be expressed and fostered by an funding policy that supports materials modelling-enabled business growth.

This document gathers the input from more than 700 interested parties on commercial end-users needs to introduce materials modelling in to their business cycle.

The discussion should establish a first list of

- key areas of company interest for materials modelling solutions and how those solutions can be achieved
- the features that would allow materials modelling to be successfully applied by companies

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.

1) Business Decision Support System

In a global context, making well-thought out decisions on which business strategy to follow and how to best serve more demanding customers is a very complicated process. It requires making choices between multiple options both on the commercial as well as the technical side of the business. A business requires, at every operational level, answers to specific questions for making decisions that



minimize risk and maximize the success rate of actions. Today, it is feasible to apply IT tools to process “big -science & technology and business- data” into smart options for data driven decision making that can strengthen the agility of companies, particularly SME’s.

Two important challenges need to be addressed to bring materials modelling to a next level of industrial use. Easy and flexible integration of existing materials models in combination with empirical information to address various industrial problems is a first challenge. Many technical challenges have a complicated multi-variable nature. It typically requires the use of multiple models, each of which may have limited applicability or accuracy. Even then, additional empirical information is often necessary to achieve realistic solutions to the challenge.

The second challenge is the combination of simulated potential technical options with the commercial decision making process. Market trends, pricing, customer needs and demands are some of the additional criteria for selecting a specific technical solution tailored to an identified process or product need.

Hence there is an industrial need for the development and implementation of methodologies for flexible integration of various materials model types adapted to industry selected challenges that in combination with business criteria define the technically possible and commercially most attractive solution.

2) Industrial requirements on software

Numerical simulation is needed to effectively and efficiently design and engineer new products, and thus minimize the need for prototyping and testing. Numerical simulation in industry is mostly dominated by Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) solved by Finite Element or Finite Volume Analysis, and forms part of the Product Lifecycle 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 mostly determined by experiments. As a consequence, the influence of the chemical material structure and its macroscopic performance in the end-product is usually missed! More and more companies have recently started using electronic/atomistic/mesoscopic materials modelling to include more detail in their simulations. With the increasing importance of materials for the European competitiveness and sustainability, it is urgent today to develop the materials modeling community and software tools and to mature these tools for an effective and efficient use across various industry sectors and application areas.

In order to use academic software codes in industry the codes should be actively transferred to third parties via licenses. It should be ensured that academic software offered freely as open source code is developed according to standards that make it operational in industrial contexts or academic software should be exploited as proprietary software owners who can also maintain the code.



Hence there is an industrial need for the development and implementation of methodologies to transfer developed materials models to the manufacturing industry. Special attention should be given to integrate electronic, atomistic and mesoscopic models into continuum models.

3) Validation

Industry has established procedures for experiments to be conducted after DIN norms and certified procedures to qualify materials for end-user applications. Industry is extremely careful to switch to new tools even if they could achieve faster and cheaper materials development processes. To improve the acceptance of materials models and model systems, validated models and model chains should be available. Credible case studies could help in their acceptance.

A database of certified models and model systems which can be used to solve specific problems or can be combined into model systems with an estimate of the error in the model prediction depending on the evaluated parameters would be welcomed.

The link between materials models and experimental tools should be established so that industry can integrate models and experiments into their materials design, optimization and validation processes and thus make the use more robust and reliable and reduce the risk of investments.

Educational test cases, showing how experimental data can be connected to simulations would be helpful to stimulate the use in industry.

4) Translators

Smaller industries will not have the expertise to execute the modelling themselves and there is a need for translators a new type of players who have the ability to 'translate' industrial problems into cases to be simulated. These players could translate material models into methodology/workflows.

"Translation Experiments" for both big companies and SME's should be elaborated as convincing dissemination material showing best practice on analyses of business cases and how they have been translated into materials simulations. A code of conduct for the translators might be helpful, similar to fields where "trust" is as important as technical competence.

5) Best Practice Case studies

What would case studies have to look like to convince manufacturers to use materials modelling in their business processes?

6) Modelling Market Place

The MMP envisions an IT system with a web front end that acts as a **marketplace** linking various activities in Europe (a central modeling hub casted as a market model). The Material Modeling Marketplace promotes an open platform designed and tailored for European industry needs



and aspires to provide fast, efficient and reliable information processing and linking of the entire material modelling activities, knowledge and competences in Europe.

The MMP will also push toward standards of simulation tools, covering models, input and output through the use of interface wrappers. Interface wrappers will be used in the general sense, that is conversion tools and libraries that can wrap existing software interfaces and libraries, and it does not refer to GUI. The interface wrappers are also meant to be applicable to both software components and databases. The aim is that mixing simulation data, experimental data and databases in the same workflow will be possible.

As such, it is expected that MAN activities will also benefit from the MMP IT platform, infrastructure, data standards and databases. Specifically:

Main benefits to industry (MAN)

- Interact efficiently with the whole materials modeling community
- Readily find partners/solutions/data/models
- Access to translators and model developers
- Ability to distinguish between validated and not validated models

These benefits are expected to lead to a strong decrease of time to market and costs of development of new products.

The MMP web front-end can offer the following resources:

- Resources:
 - Communication platform between MAN and other groups and stakeholders
 - Databases of actors (who can supply modeling solutions to MAN)
 - Case studies and white paper repositories for R&D departments of MAN
 - Expertise resource for analyzing specific problems: whether modeling can assist to solve them and how
 - Channels for education for the R&D personnel of MAN stakeholders
- Databases of:
 - Software solutions and corresponding example datasets
 - Models and data
 - Coupling and linking libraries (wrappers)
 - Open Software Tools
 - Expertise and actors

MMP will rely on input and collaboration with MAN to guarantee that the above mentioned resources and databases comply with MAN needs and therefore be of best practical use in the long run to the entire industrial sector in Europe.

The following are some of the questions and issues that could be addressed in the discussion:



What would you want to find at such a website? Data repositories? Would you be willing to share your data? Code repositories? Expertise repositories? What would your requirements be?

More specifically:

- Would you be willing to provide and share with MMP the Industrial requirements on databases of models, simulation data and experiments (validation)?
- Would you be willing to provide MMP requirements for IP management issues? How important, e.g., to have anonymous, encrypted search and query operations (and in general access to databases) for the IP of a company?
- How important are the Database of Actors, Models, Data and Validation databases to the MAN? In what form can they be of most use? What is the information you expect to have in it? And what not?
- What use can a direct communication platform, a show cases sections, a section with a collection of case studies and white papers as well as a section of educational and support resource bring and contribute to the MAN R&D workflow?
- What requirements should these resources have in order to enhance and accelerate the development process of new materials and products?
- How can standards, in the eye of MAN stakeholders, further help in exposing and exploiting the outcomes of the modelling sector to new products in industry?
- Should modelling communities /e/a/m/c/ be encouraged to use standard data for modelling and interfacing models when possible and also provide the data to the MMP for including in the databases? Do you support EU actions to this end (such as CSA)?
- Should such databases from the MAN point of view be centralized, i.e., stored locally on the MMP infrastructure or be distributed? In the later the MMP will develop standard interface wrappers to connect all databases to one repository, enabling cross-searching and correlation of data from multiple resources in a one stop shop.
- Will MAN be able to supply data to the MMP regarding typical USE CASES so that MMP can work out a set of technical IT requirements for the databases to meet better the needs of MAN stakeholders?
- Will MAN support actions directly promoting the above activities and do you support the plan of EMMC-MMP? What are the most important issues that MMP should focus on in the next 5, 10 and 15 years from the MAN perspective?
- Would a paid service be of interest to MAN? And in what form? If such a web-site is important how can it be sustained if no paid service is offered?



- Would you like to see all or most of the results of EU projects be published publicly, e.g., after a certain period? Will you want a system that controls the publicity level of the information?