Discussion Note

EMMC TRANSlators

Material Modelling: Translators Needs and Specifications

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.

Manufacturing companies across Europe (SMEs as well as large corporations) recognise the potential power of materials modelling to drive a radical change in speed of product design for and cost of manufacturability and in-use performance. Computer Aided Engineering software tools need materials models, which are a function of the previous processing history or based on data from a lower level in Multi-scale Materials Modelling (MMM) approaches.

However, modelling is not always on the critical path of commercial development because modelling tools are often seen as too difficult to use, not accurate enough, not validated for the specific material of interest and process conditions, or unable to provide answers to very specific questions.

It is well acknowledged that there remain a number of technical challenges for the development of modelling methods, tools and software for materials modelling to allow them to be routinely used in manufacturing industry. On the other hand, there is plenty of evidence that important and impactful topics can be addressed with already existing materials modelling technology. There is, however, a gap in awareness, knowledge and skills that hampers industry to unlock the potential benefit of current modelling technology. Manufacturing "end-users", in particular SMEs, quite often have insufficient expertise that prevents them from integrating the materials modelling into their development and production workflows. There is, hence, a need for new players who have the ability to 'translate' industrial problems into cases to be simulated. Consequently, a team within the EMMC, the Translators working group, has been formed with the mission to identify ways and supporting instruments of how to bridge the innovation valley of death starting from the side of the industrial innovation hill by using materials modelling and simulation. This includes the closure of the "language gap" between industrial stakeholders and scientific modellers, including training of the industrial operators during implementation of modelling and simulation at industrial R&D sites. The focus of the Translators is the industrial return on invest and the time to solution.

Translators are new actors on the scene and the role of the Translators needs to be developed fully in the future. However, from the initial definition of the Translators, it is clear that Manufacturers are the most important stakeholders for Translators. Business Decision Support Systems (BDSS) are one major requirement of the manufacturer stakeholders, so this topic needs to be addressed carefully. Since 'translation' starts from an industrial problem and ends in something to be simulated, support for a 'back-translation' of the simulation results to BDSS needs to be included into the role of the Translators.

Translators can also play an important role in the identification of the needs of industry in terms of required material models, validation ranges, availability of test equipment, parameter determination procedures, robustness of implementation etc.

First definition of the role of Translators

Translators start from an industrial problem and identify a workflow for its solution by using materials modelling. The primary stakeholder within industry interested in a modelling is usually the R&D unit, but the industrial problem is usually set by the high level management or the sales unit. In order to detail the definition of the Translators role in problem solving, it is therefore necessary to understand the industrial context of the problem to be solved, as the context defines the necessary quality attributes of a solution to a problem. These quality attributes will always include time to solution and money to be invested in order to get the solution. Savings in these two attributes are usually mandatory for the usage of modelling at all. The role of Translators includes the identification of all quality attributes, or at least the most important ones, within the language of the context of the technical industrial problem. This includes non-technical cost measures, like the influence of the solution on the pricing of a final product, and time to solution.

In order to translate the technical industrial problem to a modelling workflow, Translators need broad background knowledge of existing models and software and their capabilities. This core competence allows Translators to identify within the industrial (sub-)problems where modelling and simulation can really make a difference in terms of the quality attributes of a solution to be developed. Translators are not bound to specific models or software tools, they do their best to identify the best possible tools to be integrated into a modelling workflow.

Modelling Software tools, as to be used within the simulation workflow, may include data driven models beside materials modelling software based on predictive scientific models. Translators are aware of the fact that not every aspect of a technical industrial problem may be casted into predictive models, most often for complexity reasons. Translators develop and implement methodologies for using materials models workflows, including identification of necessary materials characterization of materials via properties or data. This may include software components connecting models operating on different scales as technical industrial problems usually call for a multi scale modelling (MMM) approach. Also important is the validation of specific models used at various steps in the process, not only to validate the tools but also to build confidence in the materials modelling at the industrial work floor. Within the implementation phase of these workflows at industrial sites, usually within the R&D units, a training guide for industrial operators using these methodologies will be developed.

Translators are aware of the fact that industrial problems to be solved by modelling and simulation are usually subject to change (and sometimes very rapid). This applies to the technical problem as well as to the industrial context. Translators support this by change management of requirements.

The role of Translators covers the “back-translation” of the results obtained by modelling and simulation workflows into the quality and cost attributes defined within the industrial context. The technical quality attributes are commonly referred as Key Performance Indicators (KPI). However, in an industrial context business related measures like pricing, time to solution and sometimes even regulatory issues are usually as important as the KPI’s.

The credibility of Translators is based on neutral support to implement the appropriated methodology independently from software or suppliers. Best practice guide, evidence on trusting, successful case studies and examples of MMM methodologies for industrial problem solving are the information provided and elaborated by Translators (in the EMMC platform) to convince, with clear neutrality, manufacturers to adopt the MMM approach.

Actions:

The actions identified so far will be carried out on a voluntary basis

A. **Develop a Code of conduct: trust is important. Since Translators need to gain insight into the context of the problem to be solved, a template NDA might be useful.**
B. **Document industrial success stories of translation efforts done for instance during project acquisition (big companies and SME's)**
C. **Retrospectively use these projects in order to identify best/worst practice communalities, set up a best practice guide for translation.**
D. **Develop draft of a methodology for the analysis of industrial problems.**
E. **Translation experiments: use Translators methodology in order to identify necessary improvements on the Translators methodology**

Business Decision Support Systems (BDSS)

Translators may assist in setting up Business Decision Support Systems and may implement software components necessary within a BDSS. This topic has been identified by the MAN group as a key industrial need and is one way to fulfil the Translators role. The setup of technical aspects of an industrial problem, which has successfully be mapped to a MMM workflow, within a BDSS is a model of the KPI's as functions (functionals) of the MMM state variables. Business oriented quality attributes may depend on the MMM state variables as well since for instance costs and processing time usually depend on the material variant currently used within the modelling workflow.

As a consequence, a business decision support system needs to be able to optimize multiple criteria. Translators advice optimization methodologies in order to solve the (Pareto-)optimization problem; i.e. identify the best possible compromises between usually conflicting quality attributes. As these solutions are usually not unique, what if scenarios could be discussed for instance between sales and R&D since "optimal" KPI's might violate business roles and vice versa, supported by visual exploration tools of the optimal compromises. It is important for Translators while setting up a BDSS to asses and reflect within their proposed BDSS setup the decision making process within the industry. This is not unique. While in large companies, with dedicated R&D, sales and higher level management, decision making involves several internal hierarchies, in SME's the decisions are quite often taken by a small and less formal group of people.

In an industrial context, irrespective of size of company, risk analysis of a decision is a common and necessary practice. While it is hard for Translators to evaluate the risk of a change of the industrial context of the problem they are working on, for the model based KPI evaluation there is a possible solution: once error estimators for the MMM states are available, these error estimators could be turned into risk estimators for the KPI's and are therefore based on materials modelling. The incorporation of business oriented quality and risk attributes call for open interfaces of a BDSS for the integration of purely business oriented context attributes by industry. However, optimization solvers using all quality attributes are an integral part of BDSS software platforms.

Moreover, the human resource investment is key business decision factor for the integration of MMM in industrial Engineering or R&D departments of the end-users/companies. The Translators supports the education of this new "figure" based on lesson-learned with basic training and training on-job.

Actions:

Suggested funding scheme of the following actions: CSA or IA.

A. **Initial design of a BDSS: workflows, best practices, Pareto-optimizers and KPI models for specific materials models and industrial challenges.**
B. **Development of a software platform for BDSS, interfaces to model software integration and convenient set up of KPI models; interface to business oriented quality attributes, multi-valued optimisation problem solvers integration.**

Software Exploitation and Models

Translators are to be considered as end users of models implemented within software tools. The basic role of Translators however calls for some specific features of software modelling tools which are important for their interaction with the manufacturers. Building modelling and simulation workflows calls for open interfaces to simulation software tools, the more standardized the better, in order to implement the workflow. The integration of these workflows in BDSS systems, i.e. for the KPI modelling, call for open interfaces as well. In particular, interplay of (Pareto-) optimization algorithms with modelling software tools works best if even the numeric used within the tools is tuneable by the optimizer, for instance convergence parameters. A solution which is detected to be far away from the optimum does not call for a full convergence of the state variables since this solution is neglected by the optimizer anyway. Even more classical response surface modelling methods may profit from open interfaces since sophisticates initialization by existing solutions of nearby problems, which leads to faster convergence, are seaming less implementable. At this level, modelling software modules as libraries with documented interfaces are superior for integration with the optimizers in a BDSS.

There are additional features of modelling software which ease the life of the Translators. Among these are State variable error estimators (via uncertainty of KPI's turned into risk assessments), Time to solution estimators for a particular run of a modelling workflow, robustness of the software and validates application ranges. Further important aspects of simulation tools are ranges of validated operating conditions for specific materials, required level of detail vs ease of robust implementation, and accuracy vs computational speed.

On the other hand, Translators may support software providers in the detection of gaps within the software tool landscape and by providing industrial relevant benchmark problems.

Actions:

Participation in the standardization and open platform actions in order to express the needs of the Translators. The needs of Translators may be casted into Use Cases of modelling software tools so that interface designs may reflect these Use Cases.

Validation

Naturally, Translators are highly interested in validated modelling software. Without validation the integration into modelling workflows is in doubt from the very beginning of a translation effort. Validation should be done against application ranges of industrial relevance; Translators may help to define such ranges. On the other hand, industrial problems might call for new materials characterisation tests. Since many models need experimental results for their initialization, Validation should include sensitivities of the Validation results against experimental uncertainties. These sensitivities may be transformed into a reliability analysis of the solution generated by modelling workflows.

Actions:

A. **CSA to develop a virtual EU platform of Laboratories able to carry out experiments and validation of models for integrated materials modelling within an industrial process chain up to product service life.**
B. **CSA to develop new test facilities/devices and experimental protocols adapted to the needs of validation.**
C. **Inverse optimisation strategy to calibrate automatically the accuracy of numerical material modelling with real experimental results taking into account uncertainty.**

Case Studies

In the long term, Translators may support case studies by providing cases and benchmark problems which include:

1. KPI models, benchmark problems
2. Strategic coverage of Industrial demands
3. Requirements of target industrial audience
4. Keywords to classify the case studies categories

Thus, the case studies proposed go beyond the usually used and academically driven case studies. Naturally, these cases studies will highlight the importance of not only covering new models, but also the importance of improvements in already existing models and software tools.

Proposed template of CASE STUDY:

1. Objectives of the industrial customer (by MAN)
    a. Free description of the industrial problem
    b. Classification of the project: material, industrial sector, scale of the material, industrial application (system, sub-system, component, fluid state, solid state, etc), weakness of actual approach (trial and error, only simplified lab experiment, no full scale model, etc)
    c. Requirements and Expected results to understand the material behaviour
2. How the Material Modelling play a key role in the problem solving (by EMMC)
3. What is the tool and methodology has been applied (one scale, multi-scale, optimization strategy, calibration of model before of iterative solution research etc.) (by EMMC)

   a. Link to SWO, MODels
4. Expected improvement of the material behaviour simulation (by EMMC)
5. Technical and technological benefits and return of the investment = satisfaction of the customer (by MAN)
   a. KPIs and ROI are part of the agreement to measure the Modelling answers vs Industrial investment and previous approach

Actions:

CSA to support demonstration and validation and robustness of the materials modelling tools.

Modelling Market Place, Outreaching

The MMP envisions a web front end, which acts as a marketplace linking various activities, communities, data, models and information throughout the material modelling landscape in Europe. As such, it is expected that all EMMC activities will also benefit from the MMP IT platform and infrastructure. The MMP web front-end can offer the following resources for, among others, the translators:

- Channels for education
- Communication platform with MAN
- Requests for model extensions
- Catalogue of existing experiments for validation purposes.
- Repositories of best modelling case studies, white papers and best modelling approaches/standards
- Databases of actors
- Expertise resource
- Databases of
  - Models and data
  - Expertise and actors
  - Coupling and linking libraries (wrappers), including Multiscale Materials Modelling interfaces
  - Software solutions
  - Open Simulations and wrappers

Actions:

In a CSA or IA, work together on the requirements and software specifications of:

- **Translators workflow**
- **Education resource and teaching actions**
- **Expertise exchange resources**