Discussion Note

SWO group

Material Modelling: Software Owner Needs and Specifications

Please state whether you agree with the following statements

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. Numerical simulation in industry is mostly dominiated by Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) solved by Finite Element or Finite Volume Analysis, 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 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.

This document gathers the input from software owners who are licensing their code, and who are thus actively transferring their software to third parties. This includes academic and industrial software owners who offer their software as open source or proprietary software owners who sell their software.

The discussion should establish

- How to gather the key representatives of the academic and industrial software owners to discuss, prioritize and communicate the needs of software owners.
- The development and implementation of methodologies to transfer academically developed materials models to the manufacturing industry. Special attention will be given to integrate electronic, atomistic and mesoscopic models into continuum models.
- How to achive that materials modeling and simulation will become an integral part of Product Life Cycle Management in European Industry, where the desired performance of the end product is met by designing the material from the electron up!

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

1) Software houses requirements on academically developed software

What can exploitation of academically developed software look like?

Extensive effort and funding has been spent in the past years on materials software developments. This software is not always exploited commercially after the end of the project. In order for industrial programmes to continue to support model development and application, the following could be done to transfer academic software to organisations which use it industrially:

- Strengthen academic - ISV collaboration; including regular meetings between academic and professional scientific software developers. Also industrial stakeholders ('expert users') should particpate. The risk of fragmentation into many small efforts should be avoided.
- An investigation should be made of existing software and the business problems the software can solve. The value proposition should be documented.
- In order for academically developed software to be employed by industry the software should be written according to certain standards which entail:
    - Reliable and accurate code.
    - Based on a reliable parameter databases which is generally accepted
    - Capable to provide as far as possible clear and unequivocal interpretation of results
    - Use of standardized file formats
- Software should be licensed with L-GPL or BSD wherever possible.
    - 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.
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- A code repository should be developed with the following characteristics
    - permanent repository and tracking of all the versions of the code, and associated reference data (e.g. pseudopotentials for first-principles planewave codes)
    - exhaustive list of examples on paradigmatic test cases, with reference inputs and outputs that need to be reproducible with machine precision
    - continuous testing on said examples, to verify that every modification of the code preserves the integrity of the results

- clearly defined and documented standards on the input and especially output data, to make it possible to integrate such software or the data it produces in more complex (e.g. multiscale, or multiphysics) frameworks
- open provenance model, where all objects in the repository are associated with a unique UUID
- validation cases, where the predictions of the codes are compared against experimental data

Hence there is an industrial need for the development and implementation of methodologies to transfer developed materials models to the manufacturing industry via licensed codes. Special attention should be given to integrate discrete models into continuum models.

2) Software houses participation in and requirements on validation

Industry requires validated models and model chains.

- The success of materials models in validation exercises can be improved by increased capabilities of material modelling obtained by
  - integration of materials models and experimental tools
  - through the building of knowledge platforms to share libraries of material parameters extracted from discrete models.
- Define a widely-accepted standardization of material parameters, avoiding the presently prevalent large variability.
- Software owners are willing to participate in public validation exercises and in 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.

3) Software houses needs on databases for applications by users

The parameters in the materials models are mostly determined by experiments. End-users of software thus often also need a database to operate the software.
The vision of SWO on the creation of such a database is……

4) Need for model development and application

SWO have identified the following gaps in industrial applicability of existing software

- true integration of atomistic with mesoscopic and continuum models.
- lack of access to computers + software by SMEs in the manufacturing industry

5) Coupling and Linking of codes

Next to the development of the IT side of linking codes there is a need for the development of the coupling and linking of models. The vision of the SWO with respect to coupling and linking is

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6) Open simulation platform

The vision of software owners on data transfer standards and an open simulation platform are

- they should be widely supported and expendable by all involved parties and hook into all different codes from discrete to continuum as well as all sorts of other proprietary software tools (database/mining, analysis, ...)
- Sustained, continuous development of the platform is essential for its broad adoption.

7) 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.

The software owners can meet these needs by the following actions:

- 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.
- …

8) Case Studies

- Educational test cases, showing how experimental data can be connected to simulations would be helpful to stimulate the use in industry.
- Tutorials on basic software usage for “standard” problems are necessary
- Credible case studies are necessary to convince end-users of the performance of the models.

- Software owners are willing to participate to the elaboration of public case studies

9) Translators

- There is a lack of expertise / usability in industry for applying modelling to the decision making processes. Inexperienced end user (e.g. small company). The impact of modelling can be increased significantly if the user base can be increased to outside a limited group of experts. For this, easy access, standardised procedures, user-friendliness, etc. may all be important. But most importantly a new player should be put in place: translators who do research for industries based on materials modelling.

10. Market modelling place

The MMP envisions a web front end, which acts as a marketplace linking various activities, communities, data, models, software and information throughout the material modelling landscape in Europe. As such, it is expected that other EMMC activities will also benefit from the MMP IT platform and infrastructure. It would be therefore important to discuss both the SWO and MMP's needs and requirements so that maximum benefit and impact can be achieved.

The MMP platform envisions the following services or sections on the marketplace:

- Resources:
  - Channels for education,
  - Communication platform with MAN
  - Case studies and white paper repositories
  - Databases of actors
  - Expertise resource
- Databases of
  - models, and data
  - Expertise and actors
  - Coupling and linking libraries (wrappers)
  - Software solutions
  - Open Simulations and wrappers

The MMP also promotes the use of standard interfaces to data, models and simulation software, or at least to have standard wrappers allowing different software tools to communicate and thus to be used to solve complex coupling and linking scenarios. These interface wrappers are not meant to replace the GUI components of a software tool, nor to be integrated by SWO themselves. It is meant as a way to allow third parties to write a new library interfacing with a tool so that the data and information can be moved from one tool to the other. This is eventually needed for e.g., for linking and coupling.

It also opens the possibility for SWO to offer their tools as components in other market segments, hence extending their outreach.

The question is, in what conditions can SWO provide specifications for their software interfaces (Application programming interface) and data structures so that interested third parties can develop wrappers and interfaces to them?

What are the requirements of such wrapper databases from the SWO point of view? Do we need two separate sections, one publicly available, another that provides information only upon request/agreement with the respective SWO who owns the specifications?

Shall specifications of software tools be treated same way as databases of simulation data and models?

What are the sections in the MMP and databases that seem to the SWO as offering the best opportunities for exploitation?

Will the SWO provide requirements for software repositories?

What should the requirements, from the end user point of view, on each of the database be so that it can be of maximum impact to SWO?

Will SWO collaborate with MMP to have a central European software repository for open source software?

How useful could it be if a certain application input/output files can be converted by means of a wrapper to input/output files of another application? Thus utilising the use of previous knowledge in new software?

What kind of requirements SWO expect from the showcases section?

Do SWO see benefit in the education, training and case studies section? What requirements are expected? Will SWO be willing to communicate them (on the technical IT level) to the MMP?

What would be the requirements and conditions on a modelbench website where specific cases are modelled with various tools, and the features and capabilities of each tool for a specific problem can be tested? Will SWO see this as a positive channel for information and outreach, or as a potential threat?

Do SWO see new opportunities of business models by integrating standard MMP database frontends into their software suits? Will SWO support such activities?

Do SWO see share the notion that the MMP will be able to give a reliable, real-time information on market demand for software solutions?

Would a “Kickstarter”-like model be of use to SWO? Example, if certain MAN stakeholders or modellers are looking for a certain feature, then they can start a “Vote” for it and by doing so commit to sponsor some of the development costs? Would a more traditional “contract” agreement be preferable? And if so how do SWO see it used in a platform such as MMP?