# Charter for EMMC team on Validation and Characterisation

## Background

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.

## Scope

This WG will support the enhancement of trust by validation of model results. 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.

## Objective

The objective for the team is to identify, define and articulate validation techniques and data that inspire trust in materials modelling or can be used as input to further develop existing materials models. Bottom-up activities and provision of policy input to funding schemes (EU, national, international,…) will be undertaken to establish and nourish an open database which enhances the usability, reliability, robustness and advancement of single models as well as model systems. The data shall be citeable by DOIs, so that the sources of this database shall be acknowledged by the community leading to a more transparent process of model validation and a fast adoption by experimentalists.

## General Goals

The **goals** for the group responsible for 'Validation and Characterisation' are to identify 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.

### Structural Goals

1. Establish a core team
2. Define a work approach and context for addressing the defining challenges associated with the objectives
3. Develop a (representative) social network on validation and characterisation of materials modelling
4. Identify together with other work groups significant industry challenges in the context of EU and international megatrends
5. Identify, define and articulate specific topics that need to be addressed
6. Formulate approaches for addressing the identified challenges
7. Document the general industry feedback, topical interests and implementation approaches for delivering input for future funding programmes (e.g. in the context of Horizon 2020.)

### Desired outcome:

The outcome of 'Validation and Characterisation' shall be a document of general requirements for an interconnected database with easy to use front ends allowing users (scientists, engineers, managers in industry companies, students and educators, etc.) to search and obtain information on the experimental validation of models and model systems, their integration into a simulation workflow and expert networks. The repository shall enhance the visibility of researchers through the possibility to cite experimental data and techniques and therefore enhance transparency. The effort will contribute to the reduction of costs and resources to develop new materials in Europe especially in case of novel materials made available by nanotechnology.

## Timeline:

Continuously: Expanding database to reach a representative social network with active core (the team)
Sept 2014: First draft as discussion paper for Nov meeting by core team
October 2014 Invitation to Nov meeting of active contributors by EC
Nov 2014: Report on outcome of the wide consultation
Dec 2014: Second version