Charter for EMMC working group on Coupling and Linking of Models

Background and role of the WG

Within the European Materials Modelling Council (EMMC), working groups (WGs) focusing on selected topics have been formed to help increase the impact of materials modelling on the European economy and society. This will be achieved by promoting quality development and the efficient use and organisation of existing and future resources in the field of materials modelling (i.e. models, methods, software and modelling infrastructure). The EMMC should also advise the European Commission in matters relating to modelling and provide input for future EC strategies, visions and plans.

Materials simulation activities are traditionally categorised according to the "smallest" entities described by the mathematical equations that are solved: electronic, atomistic, mesoscopic and continuum (macroscopic) models (e/a/m/c). Practical devices increasingly rely on materials that are engineered at the nanoscale to control electronic processes in order to achieve the required functionality. This requires approaches beyond the state-of-the-art of isolated communities in order to provide the required support for materials and device design for future industrial products in Europe. Coupling and linking the efforts within the e/a/m/c communities will create a stronger European modelling community.

The report "*Preparation of a LEIT Materials Modelling Policy*" from the 27 February 2014 LEIT meeting in Brussels highlighted that, among end-users and manufacturers, the most frequently mentioned modelling issues in need of attention were "Reliability", "Integration of models and codes", and "Validation & References". The *Coupling and Linking of Models* WG focuses on the first of these: the development of linking and coupling schemes to realise models with sufficient predictive power to be reliable replacements for expensive or unfeasible experiments in industry. The root of the problem is that *it is not yet well known* how best to couple and link different models between, or within, the e/a/m/c chainin a satisfactory way. For example, in linking e- and a-type models "upwards" for a certain material, it is usually not known which of the physical and chemical features of the electronic model that need to be carried over to the atomistic model to preserve the crucial elements of the description, nor what model expression is needed to capture these features. Going in the other direction ("downwards") is often even more problematic, with a range of possible approaches for reconstructing the missing information. The linking thus often contributes to the accuracies in physical properties resulting from the modelling of complex materials. This is particularly serious when reliable modelling results are needed for the growth of European industry.

To change this situation, dedicated development efforts of advanced physics-based models and schemes are needed, which are targeted at materials and processes of industrial use.

Scope of the WG

The WG aims to promote the targeted development of reliable combined models (coupled and linked) that go beyond the capabilities of the individual e/a/m/c models. A few examples of such approaches are (upwards) coarse-graining, systematic model reduction, thermodynamic moments mapping, filtering; (downwards) most likely states identification, entropy/entropy production maximization, thermodynamic equilibrium relaxation, lifting.

The validation of the models is clearly a closely connected issue, as is the practical implementation (coding) of the various linking and coupling schemes. Thus fruitful interactions with both the Validation WG and the Open Simulation Platform Concept WG are expected.

Objectives

- To push the boundaries of materials modelling closer to realistic applications.
- To encourage and promote the targeted development of more reliable coupled and linked models for materials properties and processes over a wide range of problem scales.
- To promote the awareness of the whole modelling chain among different categories of actors and stakeholders, and of its need for dedicated efforts and support.
- To foster interactions with the e/a/m/c communities and with the Validation and the Open Simulation Platforms WGs.
- Act as a sounding board and participate in European consultation initiatives.

Goals

- Define the main challenges associated with the objective.
- Establish short-term and long-term working approaches towards the objectives.
- Establish a core team and develop a (representative) network of engaged actors in the Coupling and Linking WG.

Desired outcome

Reliable chains of materials models with quality output for the industry.

Timeline

- Completion of a Road Map by end Q1 2015
- Continuously: Expanding database to reach a representative social network with active core team
- October 2014 Invitation to Nov meeting of active contributors by EC