The European Materials Modeling Council

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 have been 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) (see, for example, the FP7 "Modelling review" (http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html) Despite many years of effort in multiscale modelling, there are still quite separate communities and sub-communities representing these diverse models, and many gaps in our ability to connect models across the four categories.

At the same time, current and future products increasingly rely on materials that are designed and engineered at the nanoscale 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 across the e/a/m/c communities will serve that purpose and help to 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 [see definitions of the *coupling* and *linking* concepts at the end of this document] will help to address 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. *This is not possible today.*

Thus it is well known that, at least as far as available electronic, atomistic and mesoscopic models are concerned, physical properties resulting from the modelling of complex materials often carry large "error bars". This is particularly serious when reliable modelling results are needed for the growth of European industry.

A major factor in 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.

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

Scope of the WG

The scope of the WG encompasses two main tracks of modelling efforts: on the one hand, the improved and wider exploitation of *existing* coupling/linking models and schemes, and on the other, the development of *new, more accurate and robust* schemes. In a targeted LEIT context, sophisticated coupled models have an increased possibility of producing predictive results of direct industial use, but few such models exist as yet. To change this state of affairs is the overarching objective 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 individual e/a/m/c communities and with the Validation and the Open Simulation Platforms WGs.
- To act as a sounding board and participate in European consultation initiatives.

Goals

- Define the main challenges associated with the objective.
- Establish a terminology which is clear and has wide stakeholder acceptance.

- 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

To fulfil the objectives.

Timeline

- October 2014 Invitation to Nov meeting of active contributors by EC
- Working Group Meeting on 5/6 November in Brussels
- Overview of linking/coupling schemes used in current FP7 modelling projects
- Completion of a first Road Map by end Q1 2015
- Continuously: Expanding database to reach a representative social network with active core team

Team members

Kersti Hermansson, Uppsala University
Pietro Asinari, Politecnico di Torino
Roy Chantrell, The University of York
Adham Hashibon, Fraunhofer IWM
... and more to join

Appendix: Definition of Coupling and Linking

Connections between models and scales have been described in various publications and include terminology such as concurrent, sequential, hierarchical, tight, loose etc. In this Charter we use the following terminology:

Coupling: Two different but dependent physics/chemistry models are solved together, also often referred to as concurrent modelling
http://www.scholarpedia.org/article/Multiscale_modeling#Concurrent_multiscale_modelling

Linking: Linking in general is a looser type of coupling of independent models. It includes sequential multiscale modelling where information from a lower scale is passed to the model at a higher scale, but also includes linking models at the same scale, often also referred to as sequential modelling.

A major issue in linking models is the reduction, extraction and transfer of data from one model to another, all challenging processes which generally involve significant insight into the physics/chemistry of the models involved.