The European Materials Modeling Council

Charter for EMMC working group on *Atomistic 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 modelling quality development and the efficient use and organisation of both 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.

Currently most industrial materials and device designs rely on the use of continuum or mesoscopic approaches. However, with materials and devices increasingly being engineered at the nanoscale to achieve the desired functionality, the use of models with atomic resolution is becoming increasingly important. Atomistic models are semi-classical, typically relying on classical equations of motion to predict dynamic behaviour with, wherever possible, Hamiltonians parameterised from ab-initio information. The archetypal example is Molecular Dynamics (MD) using potentials determined by ab-initio calculations with some approximation such as the embedded atom method, which assumes that the crystal energy is the sum of a pair-wise potential and an energy required to embed an atom into a local medium with a given electron density. This type of formalism is typically used, in addition to providing atomic level investigations, to calculate bulk properties for use in mesoscopic and continuum models. In this sense atomistic models provide an important link between ab-initio and mesoscopic/continuum models.

In order to develop such models as a serious computational tool for materials and device design and to integrate them into the industrial environment it is necessary to develop more efficient code and to extend the domain of application by merging atomistic and mesoscopic/continuum models. For example, Finite Element Method code often includes the possibility of adaptive meshing in areas requiring greater computational resolution: it is necessary to consider the condition that the mesh size becomes comparable to material lattice sizes. At this point the continuum formalism used by the FEM will certainly not be applicable and the question is how to formulate an approach introducing atomistic – level approaches where appropriate. Another example is given by the opportunities offered by the reactive force fields (e.g. ReaxFF) to model chemical reactions which imply continuous bond formation/breaking.

Within this context there exists a need for a forum in which priorities for model development and discussion with potential industrial end-users with the aim of creating a European atomistic modeling community enabling the development of models capable of supporting nanostructured materials and device design. This is the pivotal role of the atomistic WG.

Scope of the WG

The overall goal is to establish an EU-wide atomistic modeling community with strong links to industry so as to facilitate the rapid inclusion of atomistic level approaches into the design toolset available for advanced material development and prototyping.

Objectives

- To push the boundaries of atomistic-based materials modelling closer to realistic applications (e.g. by including reactive force fields).
- To develop an interaction with other established organizations of the atomistic modelling community, such as CECAM.
- To foster interactions with the electronic and mesoscopic/continuum communities and with the Coupling and Linking Models WG as well as with the Validation WG.
- To act as a sounding board and participate in European consultation initiatives.

Goals

1. Establish a core team

2. Define priorities for model development.

3. Establish the current user group and its model usage.

4. Initiate and develop a dialogue with potential industrial users.5. Completion of a Road Map for integrating atomistic models into industrial product development.

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
- Completion of a first Road Map by end Q1 2015
- Continuously: Expanding database to reach a representative social network with active core team

Current team members

Kersti Hermansson, Uppsala University
Roy Chantrell, The University of York
Pietro Asinari, Politecnico di Torino
... and many more