European Materials Modelling Council (ECMM)

Charter of Continuum Models Group

Background

The European Materials Modelling Council (EMMC) is a bottom-up organization started in February 2014 by the Advanced Materials & Nanotechnology unit of the Leadership Enabling Industrial Technologies (LEIT) programme. The objective of EMMC is to connect all activities happening in the field of materials modelling. The EMMC is divided in working groups (at present time 16) and the WG Continuum Models (CM) is one of them.

The Review of Materials Modelling, Chapter 4, describes the continuum models. A short extract is given here. This type of models is a wide category based on the continuum hypothesis being adapted to describe the macroscopic behavior. The length and time scales of CM are larger than the typical scales of electronic, atomistic and mesoscopic models. In contrast to CM, the Review of Materials Modelling, describes electronic, atomistic and mesoscopic models as discrete. Materials continuum models can also deal with peridynamics, deformations with discontinuities, especially fractures when applied to continuum scales. The general structure of models is based on balance equations (e.g. stress and strain, momentum, energy, mass), constitutive laws, sometimes evolution laws (e.g. for take in to account phase transformations) initials and boundary conditions.

The CM can be applied to describe physical phenomena in different fields: solid mechanics, fluid mechanics, heat flow, continuum thermodynamics, chemical reaction and diffusion, microstructure evolution, electromagnetism, materials manufacturing processes and materials behavior in devices. The microstructure evolution, by CM point of view is strongly correlated with the materials properties (e.g. mechanical, thermal, electromagnetic) at the continuum scale. Moreover, microstructure evolution can be modeled both with continuum and with discrete models so that provides the natural link between continuum and discrete models. These fields are often coupled, classical examples are the fluid-structure interaction, thermo-mechanics and thermo-electromagnetic models and this is usually referred to as multi-physics models. Through this coupling the models find wider application; e.g. thermo-mechanics or thermo-electromagnetic-mechanics models which can describe microstructure evolution and much more. It can happen that the phenomena described by multi-physics models have very different time scale, e.g. in a thermo-electromagnetic simulation there are three orders of magnitude between the time scales of the thermal and electromagnetic fields.

The CM cover a plethora of applications in all the fields of the engineering, natural sciences, biomedical sciences, material science etc. On the other hand, these models are not yet used to their full potential (mainly industrials, but not only). The important reasons seem to be:

1. the possible users have no an adequate knowledge of continuum models possibility;

2. often it is very hard or expansive to obtain the continuum models parameters (particularly, appropriate materials characterizations);
3. the experimental validations can be very hard or expansive.

Scope

The general scope of the Continuum Models working group is to enlarge the applications the CM and to influence their development. The CM working group aims to become a neutral meeting point among users, model and tool developers of continuum materials models. This WG wants to provide a wide view on the existing knowledge of modellers, tool availability and needs of users. Concerning the software tools, all types (commercial AND academic; "Open source" AND "black box") will be considered.

Increasing the number of CM users will be based on the following actions:

1. To make and publish a survey on the existing continuum models;
2. To select and to propose to possible users "Frequently Asked Models" (continuum) that can meet the need of many applications.
3. To encourage the model developers to adapt the models to the needs of possible users, particularly industrial users.
4. To encourage the experimenter to adapt their characterizations to the need of continuum models.
5. To link continuum and discrete models (parameters and materials properties obtained by discrete models should be used in continuum models)
6. To encourage the publication of materials properties and characterization needed for CM, particularly those financed by public institutions.
7. To encourage the publication of experimental findings that can be used as reference to validate CM, particularly those financed by public institutions.

The industry requests continuum modelling chains for virtual manufacturing, components design and the prediction of components life performances (e.g. fatigue and wear). The EMMC WG on CM will try to find and close the gaps in the respective modeling chains. Moreover, the WG will try to close the materials properties gaps especially by integration of discrete models (electronic, atomistic and mesoscopic) with the continuum models and by encouraging the publication of materials characterization data.

The WG will further provide all the action necessary to promote the integration of the results of multi-scale non continuum models into CM.

In order to influence future CM development, the WG will provide inputs for future visions/plans for funding agencies based on the acquired knowledge on user needs, possible models development and on technical and scientific gaps.

Objective

The objective of the Continuum Models working group is to enlarge the use of the existing continuum models and promote their development as well as the elaboration/promotion of new CM where applicable. Integration of discrete models with continuum models will be promoted and awareness campaigns for industries will be undertaken.

Goals

1. Establish a core team and organize the sub-structure of the group;
2. Develop a (representative) social network among stakeholders, users and developers (models and tools) adequate to become a reference point for anyone working with CM;
3. Define a work approach and context for addressing the emerging challenges associated with the objective;
4. Elaborate a set of case studies, Frequently Asked Models (FAM), of typical industrial processes, components design and component life performance that can be used to demonstrate the benefits of continuum materials modelling and its integration with discrete materials models;
5. Interact with other WG on the specification of communication data standards appropriate to for the development and the applications of CM;
6. Interact with the validation WG in order to increase the credibility of the CM;
7. Provide strategic inputs for future vision/plans.

Desired outcome:

Wide industrial awareness of the benefits of existing CM (integrated with discrete models) and stimulation of further development of CM.

Timeline:

- Continuously: expand representative network of stakeholders with active core;
- Continuously: collect information about availability of CM, tools and user need;
- Continuously: collect information on the integration of CM, tools and user need;
- October 2014 Invitation to Nov meeting of active contributors by EC
- Nov 2014: Report on outcome of the consultation in Brussels

- Dec 2014: draft Road Map for CM WG

Current team members

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