The European Materials Modeling Council

Charter for the "*Discrete models WG*" within the EMMC

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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. In this context it is important to consider the long timescale of model development in the discrete modelling community.

Time is a key aspect to the Discrete models WG in at least two ways, namely, on the one hand, the time- and length scales possible to reach within discrete-models simulations, and on the other hand, the time-scale that is needed for the development of a discrete model of a high enough quality (i.e. containing the sufficient and necessary amount of the relevant physics and chemistry) to be of use in industrial and other key applications. When such realistic models with a predictive capacity are sought, the timescale required from concept to model verification against experiment can be 5-10 years, while industrial timescales are generally much shorter. The Discrete Models EMMC recognises this difference. Sustainable and continuous efforts, and the enabling means, are needed to achieve the necessary development of materials models and the widening of their applicability. There is thus a pressing need for continuous support of long-term model development at the discrete lengthscale; an area of considerable European strength.

As far as simulation time- and length scales are concerned, there is an increasing need for *tailored* materials design at the electronic and atomic/molecular levels and there is also a growing use of complex nanostructures that provide new or enhanced functionality, with an entailing need to understand, predict and design such *tailored* functionality at the nanoscale. However, Numerical materials simulation in industry today is nevertheless to a large extent dominated by Structural Mechanics (SM) and Computational Fluid Dynamics (CFD) modelling solved by Finite Element or Finite Volume Analysis, i.e. simulations "high up on the multi-scale ladder". The parameters in the SM or CFD models are mostly determined by experiments. As a consequence, the influence of the chemical material structure and its macroscopic performance in the end-product is usually missed! Such detailed information becomes particularly critical when the materials properties and processes depend *explicitly* on the material's behaviour at a very fine-grained level, such as the very small active chemical sites in the multi-billion dollar catalysis industry. Currently most industrial materials and device designs rely on continuum or mesoscopic approaches, but 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.Ggradually more and more companies have realised the importance of using discrete materials models, i.e. electronic, atomistic or mesoscopic materials modelling, to include more detail in their simulations.

The discrete models WG deal with most aspects of improving and promoting electronic, atomistic and mesoscopic (e + a + m) materials modelling in Europe, as well the coupling and linking (C/L) of these models, all this with particular focus on the industrial context. This WG will give a stronger voice to the "discrete-models" modelling communities towards overcoming difficulties in penetrating industrial practices at large, and a stronger voice in the discussion with other stakeholders in the EMMC.

The Discrete-models communities

The *electronic structure community* is one of the largest communities of modellers in Europe, both in terms of number of actors and HPC usage. Both wave-function based and DFT-based models belong here, as do the various approaches to exploration of the potential energy landscape and methods for advanced property calculations. Information from electronic structure calculations, i.e. quantum-mechanical (QM) calculations, is required in a range of situations where the detail of electronic models is needed, or where data of the accuracy of high-level QM calculations is needed. This may concern the information about the most likely route for a chemical reaction, the consequences of defects in a material, the relative stability of crystal polymorphs for use in pharmaceutical industry, or the design of more powerful magnetic materials. In addition to such examples where materials properties and processes depend explicitly on the behaviour of the electrons (the electronic wavefunction) or their energy levels and spins there are a number of other circumstances where QM calculations are needed. One example is the generation of ab initio-derived quantities that can directly be used as parameters in more coarse-grained or continuum models, typically when experimental parameters are not available. Another example is the generation of data that can serve as a training-set for the parametrization of more coarse-grained interaction model (e.g. e => a), or the reverse procedure, when some interesting phenomena or structure "observed" using an atomistic-model simulation needs to be scrutinized at the level of detail given by an electronic model

Atomistic models are semi-classical, typically relying on classical Newton 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, ???, to calculate bulk properties for use in mesoscopic and continuum models. In this sense atomistic models provide an important link between electronic and mesoscopic/continuum models (continuum will be abbreviated 'c' below).

The mesoscopic modelling community involves quite a heterogeneous and broad range of competences and/or backgrounds. Mesoscopic models describe the behaviour of nanoparticles and grains, molecules or part thereof (groups of atoms), and with these models phenomena can be described at meso length scales (nm) up to macro scales (mm). Such models, as they are of the supra-atomic type, average out less important structural details or fast details of the atomic motions or replace them by mean-field characteristics (dielectric constant, Debye length, viscosity, friction coefficient) and stochastic terms. Examples of mesoscopic models are discrete thermodynamics models where the interaction between grains and their environment (atoms, other grains, etc.) are described. Also the so-called coarse-grained version of molecular dynamics falls in this category and here the fundamental unit is a "bead" that interacts with other "beads" or atoms via effective soft potentials. This type of models can also be developed for colloidal suspensions of nanoparticles, also

called nanofluids, and bio/medical materials to describe drug delivery in humans and animals. A third subset includes magnetism models based on macro-spin approaches that combine atomic spins into a macro-spin. Mesoscopic models are used to describe the behaviour of materials but also material processes, like manufacturing processes, catalysis, synthesis, cell growth, etc.

"*Coupling and Linking of models*" efforts within our communities typically focus on the development of linking and coupling schemes to realise model workflows that can simulate phenomena at large size and time scales while simultaneously preserving, or reflecting, some of the valuable finer details of the physical system. However, it is not yet well known how best to couple and link different models between, or within, the e/a/m/c chain in a satisfactory way. For example, in running an e-type model and then link this to ana-type models ("upwards" linking) 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 material relation is needed to capture these features. Going in the other direction ("downwards") to simulate finer details of problematci areas indicated inth cosre level simulations, is often even more problematic, with a range of possible approaches for reconstructing the missing information.

Objectives and action plan

Vision:

European materials-based industries need to have access to models and modelling workflows of a high enough quality, reliability and predictive power such that modelling results will make an economical, environmental or societal difference. Therefore it is important for this WG to, on the one hand, promote the improved and wider exploitation of *existing* models and workflows, and on the other, promote the development of *new, more reliable* (yet computationally feasible) models and workflows.

Objectives:

1. **Prepare for future call texts and inventory of current model needs.**

   Create an application/industry-endorsed input on the topic of widening materials models in the coming H2020 calls. A few potential topics of such dignity and importance are the following concrete areas:

   * Models and modelling workflow for predictive design of (nanostructured) interfaces for e.g. heterogeneous catalysis or energy applications.

   * Physics in linking of e and a/m models: Development of advanced force-fields for smart and functional materials.

   * Models that manage to describe how defects make chemistry as well as physics.?????

   * Models related to quantum, electronic and spin based information storage and manipulation.

   * Too generic….

   This is only a sample list which will be modified and expended via consultation with the industrial end user community and major actors in the discrete models field.

2. **Drive strategic modelling discussions and activities.**

   The models and the modelling workflows are at the very core of modelling should have a central role in the EMMC. Members of the Discrete Models working group are very familiar with the

complexity and difficulty entailed in the concept "predictive modelling", and the considerable obstacles that need to be overcome to reach there; this needs to be articulated in a strategic fashion. The EMMC, and the Discrete Models WG, should thus take an active part in, and help drive, this strategic discussion, in synergy with the other strong modelling organisations such as Psi-k, CECAM, and EUMAT.

The Discrete Models WG should also act in synergy with the discrete models developments taking place on the international arena, and help to promote joint international efforts.

All in all, the Discrete-models WG should work forcefully towards Europe overcoming the bottleneck expressed in the Introduction (the lack of available high-quality models) and towards making visible the *pressing need to harmonise the timescales between the model developers and industrial needs and the pressing need to provide for continuous support for long-term discrete model development; an area of considerable European strength*.

3. **Enhance the discrete-models WG's interactions with other groupings and stakeholders of the EMMC.**

   There is a continuous need to strengthen the communication, interoperability and consensus among the various stakeholders and WGs of the EMMC. For the Discrete-Models WG this ambition particularly concerns the Industrial Advisory Committee, the Continuum models WG (which is the remaining Modellers WG so therefore clearly very important to us), the Translator WG (for obvious reasons), the "Software owners" WG (which should represent an obvious – and experienced – link to the end-users), the Validation WG (in fact we should jointly promote quality issues), the MMP WG (Materials Model Marketplace WG; which relies on the generation of good-quality data from good-quality models), the Open Simulation Platform WG (who should implement the C/L recipes). Clearly, the responsibility to achieve such fruitful interactions is mutual.