Charter for EMMC working group on Mesoscopic Models

Mesoscopic models for effective materials modeling

Background

Within the European Materials Modelling Council (EMMC), working groups have been formed to focus on a certain group of stakeholders. This team focuses on mesoscopic models. "Mesoscopic" is a concept used differently by different communities. In the European Commission's Review on Materials Modelling, an attempt is made to bring all models together in one unified classification and with one vocabulary[1]. Two essential features characterize a mesoscopic model and distinguish it from both atomistic and continuum models, namely (i) atomistic details are averaged out and (ii) they are applied to simulate structures with characteristic sizes for which macroscopic parameters usually do not change significantly. For example, mesoscopic models describe the behaviour of nanoparticles, grains and dislocation clusters. These models can be used to describe phenomena at meso length scales (nm) up to macro scales (mm). Fast details of the atomic motions arer replaced by mean-field characteristics (dielectric constant, Debye length, viscosity, friction coefficient) and stochastic terms. The mesoscopic model allows highly efficient and detailed description of objects and structures which sizes are still much smaller than macroscopic length scales, over which macroscopic materials parameters (density, conductivity, thermal expansion coefficient, etc.) and external drivers (temperature, pressure, electric and magnetic fields) vary significantly.

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. The EU Framework programmes and other funding schemes have contributed to develop the field and this EMMC working group would like to build on this state of the art and focuses on activities still necessary to integrate mesoscopic models into existing

[1] http://ec.europa.eu/research/industrial_technologies/pdf/modelling-review_en.pdf

modeling approaches and to transfer these models to companies, particularly SMEs, in order to stimulate the development of novel materials and products.

Scope

Mesoscopic modeling involves a quite heterogeneous and broad range of competences and/or backgrounds. There is a strong need to develop an exhaustive **survey** of different mesoscopic approaches, to understand the key underlying ideas and to highlight their advantages, limits and drawbacks. There is a need to recognize qualitatively similar ideas and modeling approaches, to identify overlaps, and to identify complementarities, in order to fully explore the potential and to get sufficient recognition. Also a common language of formulation might be needed.

Companies need effective tools to develop real products, and this requires challenging scale-ups of the software codes. Mesoscopic approaches have attracted a considerable interest in the recent past, as a viable short-cut towards more realistic simulations, when brute force, i.e. larger computational power, is not enough to do simulations with atomistic models of the required scale. However not all are yet aware. The reason lies in a mismatch between the actual industrial needs and the feasibility of the available solutions. Hence there is an extremely urgent need for a precise **map**, relating applications in terms of time scales and length scales and available modeling approaches, tools and numerical codes. This map would allow one to recognize missing gaps and to identify effective research directions.

Accordingly the scope of the work group entails: Identification of key approaches underlying different mesoscopic models (survey) and identification of their potential to meet industrial needs for some sets of specific products (map).

Participants will be modelers and software houses. Industrial manufacturing companies will be contacted to specify their needs and will thus drive the activities.

Objective

The objective for the team is to identify, rationalize and compare different mesoscopic models and to cast them in the context of making materials modeling an integrated part in industrial processes. Bottom-up activities and provision of policy input to funding schemes (EU, national, international, etc.) will be undertaken.

Goals

1. Establish a core team
2. Define a work approach and context for addressing the defining challenges associated with the objective

3. Develop a (representative) social network on mesoscopic models
4. Identify significant overlaps and complementarities in the existing mesoscopic models (survey) and how they fit in a bird-view scenario
5. Identify industrial challenges in the context of EU and international megatrends (map)
6. Identify, define and articulate specific topics that need addressing for integrating existing mesoscopic models for materials for solving industrial challenges
7. Formulate approaches for addressing the indentified challenges and ways for implementation
8. Document the general academic and industry feedback, topical interests and implementation approaches for delivering input for future funding programs (e.g.in the context of Horizon 2020).
9. Completion of a Road Map for integrating mesoscopic models into industrial product development.

Desired outcome:

The critical outcome of the team effort is the completion of Road Map for encouraging integration of mesoscopic models for materials into solutions for industrial challenges, delivering a direct impact on the competitiveness of the EU industry base. Start of bottom-up activities if necessary.

Timeline:

- Completion of a Road Map by end Q1 2015
- Continuously: Expanding database to reach a representative social network with active core team
- Sept 2014: First draft Road Map as discussion paper for Nov meeting by core team
- October 2014 Invitation to Nov meeting of active contributors by EC
- Nov 2014: Report on outcome of the wide consultation
- Dec 2014: Second version Road Map

Team members:

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Current list of identified mesoscopic models (to be completed)

1) Coarse-grained Molecular Dynamics models
2) Discrete Lattice Dynamics models
3) Statistical Mechanics mesoscopic models
    - Lattice gas automata (CGA)
    - Lattice Boltzmann method (LBM)
    - Dissipative Particle Dynamics (DPD)
    - Smoothed-particle hydrodynamics (SPH)
    - Discrete Phase Field (DPF)
4) Micromagnetic mesoscopic models
5) Mesoscopic models of dislocation networks in crystals

- The concept of materials includes also fluids, e.g. colloidal suspensions of nanoparticles, also called nanofluids, and bio/medical materials, e.g. those for drug delivery in humans.
- The models concerned can describe the behaviour of materials but also material processes, like manufacturing processes, catalysis, synthesis, cell growth, etc.

Topics to address:

- Identification of redundancies and complementarities in existing mesoscopic models
- Identification of industrial needs with regards to mesoscopic models
- Identification of scientific challenges of mesoscopic models
- ...