



Charter for EMMC team on Interfacing to HPC

Background

Within the EMMC subgroups have formed to focus on a certain group of stakeholders. This team focuses on advantages offered by peta-scale high performance computing (HPC) for advancing materials modelling. Recently new developments have been made in computational technologies for processing experimental and modelled/simulated data, which are expected to provide platform (computational environment) for solving large-scale computational demanding problem such as those involved in modeling of new materials and processes.

Many phenomena in materials have a complicated multi-variable nature, which typically requires the use of various-scale models, with the uncertainty related to transferring of variables between the scales. Additional empirical information is often necessary to achieve realistic solutions. The analysis of data quality from different empirical databases is a cumbersome procedure, which often delays the speed of simulations.

Materials modeling will benefit from recent advances in HPC by a closer collaboration between the community of modelers and the community of computer scientists who can develop specific computing architecture that meets the needs of material modelers.

Scope

The scope of this EMMC HPC work group entails: Review of existing methodologies for flexible integration of various materials models adapted to industry and transferable to massively parallel computing architectures.

Participants will be modellers, mathematicians, computational scientists, high-tech companies end-users.

Objective

The objective for the team is to identify, define, articulate and execute the necessary interfacing between the materials modelers world to the HPC world with the objective to further develop the industrial use of materials modeling. The EMMC HPC team will discuss with HPC developers what specific actions should be undertaken in order to speed up computations of complex materials and increase the accuracy of computations. A professional selection from multiple options available for deployment of materials models will be made by the team to facilitate the discussion.

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 interfacing materials modelers and HPC developers.
4. Identify, define and articulate specific HPC topics that need addressing for integrating existing materials models with experimental data
5. Document the general industry feedback, topical interests for delivering input for future funding programmes (e.g. in the context of Horizon 2020, DG CNECT.)

Desired outcome:

The critical outcome of the team effort is continuous communication between HPC developers and Materials Modellers on HPC possibilities and needs

Timeline:

Continuously: Expanding database to reach a representative social network with active core (the team)

Oct 2014: First draft of a 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: Communication of needs to HPC world

Topics to address:

HPC needs for all models mentioned in the review of materials modeling

http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html

HPC needs related to interfacing with experimental data.