

Coupling & Linking of models towards industrial needs

Introduction

Detailed modelling of physical phenomena inherently embeds dealing with different length and spatial scales, which in some cases become disparate. This multi-scale nature must be properly addressed for accurate modelling; however, accurate representation leads to stiff systems, causing a dramatic limiting factor for the numerical solution with standard methods (e.g. very small time-steps and/or very fine spatial discretization). This problem finally hinders modelling advancements for engineering and industrial applications; therefore, multi-scale methods able to address and overcome this limit are desirable. With this purpose, methods using Coupling & Linking (C&L) strategies have been - and are being - developed, together with and in parallel to model-reduction techniques (ROM, Reduced-Order Modelling). The aim of this session is to provide an overview of the currently available techniques for C&L and ROM, and their potential in industrial applications.

Objectives

The objective of this session is to discuss a Roadmap for the perspective development of novel Coupling and Linking (C&L) methods beyond the existing ones. To this purpose, the theoretical infrastructure which is needed for the coupling and linking of discrete (electronic, atomistic, mesoscopic) and continuum models will be reviewed.

- Collect feedback on and discuss the state-of-the-art C&L methods
- Discuss the limits limiting factors for current C&L and identify margin for improvement
- Discuss the industrial applicability of such methods and their potential benefit

Background information and documents

Relevant information for this session can be found in the following documents:

- The Review of Materials Modelling (RoMM) 6, which provides the required vocabulary and classification for models and workflows.
<https://publications.europa.eu/en/publication-detail/-/publication/ec1455c3-d7ca-11e6-ad7c-01aa75ed71a1>

Discussion points and questions

The following questions summarize the issues for this session.

- In your opinion, which are the most important current gaps to be filled with regards to C&L methods? Where to put more effort: discrete-discrete, discrete-continuum?
- About wide adoption of C&L methods in industry: which are the most relevant limiting factors? Lack of specific expertise in R&D departments? Lack of success stories about the benefits of adopting these techniques? Unawareness of their potentiality?
- In your opinion, which are the most relevant industrial sectors that may particularly benefit of C&L methods? Why? Which are the most relevant and urgent phenomena to tackle via C&L methods?

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- About strengthening the collaboration and cooperation between the academic model developers and industrial researchers: how can synergy on C&L method development and application be promoted to achieve a win-to-win situation?
- Do you think that a more systematic V&V layout would boost industrial application of C&L methods? In your opinion, is V&V a critical issue for widespread use of C&L in industry?