Session 5   Discussion Notes

Open Modelling Frameworks

Introduction

A large number of well-established integrated simulation environments exist, including commercial closed systems, commercials systems with APIs and open source environments. However, there is a lack of truly open modelling frameworks that enable end users to integrate any modelling, pre or post processing tools on a widely agreed, open standard footing for all types of models (electronic, atomistic, mesoscopic, continuum). At the very heart of an open modelling framework is the Open Simulation Platform (OSP) which is formulated as a set of common standards and related tools that form the basic environment on top of which compatible and compliant simulation workflows can be developed and run.

Characteristics of an OSP:

- The foundation of an OSP is an open semantic standard described in an ontology, such as the EMMO.
- An OSP enables the integration of codes into a simulation workflow.
- An OSP supports all aspects of a simulation, including pre-and post-processing and computational representations of models (including solvers).
- An OSP provides standards for the basic communication (metadata) between the varieties of components and software tools in a simulation workflow. The communication and data standards must be compatible with the ontology.
- Different levels of linking and coupling can be supported by wrappers.
- An OSP itself is separate from any pre-/post-processing or modelling codes or applications
- All information exchanged through the OSP must be represented with an ontology-compliant standard

Objectives

The objectives of Session 5 are to present and discuss approaches to open modelling frameworks and find common widespread support for the concept of an OSP. We need to find ways to link all models and databases openly as even today a large amount of data is still transferred manually or in non-standard means.

Background information and documents

- IntOP2018: EMMC-CSA Workshop on Marketplaces and Interoperability
  https://emmc.info/events/intop2018/

Discussion points and questions

- What modelling frameworks, open or otherwise are the most important ones to you and your community/organisation?
- What kind of standardisation is needed to use an OSP for interoperability?
- How would you want to use an OSP to fully automatize data transfer between models?
- Is full flexibility with tools that can link to it important to you?
- What would an OSP have to offer so that you would use it regularly?
- What would an OSP have to offer so that you would enable your software to link to it?