Session 13   Discussion Notes

Innovation hubs: foundations of modelling services

Introduction

Digital Innovation Hubs (DIH) are eco systems that consist of small and large industries, start-ups, researchers, accelerators, and investors that aim to create the best conditions for long term business success for all involved stakeholders. DIH are focused on enabling and delivering digitalization and innovation capabilities to all by means of providing focused and customized central access to a multitude of relevant services providing a better framework for the digital industrial revolution.

Innovation Hubs are meant to be essentially one-stop-shops that enable all stakeholders including small and large industries, software owners, modellers etc., to access, obtain and deploy and implement modelling services more rapidly. The goal is that companies become more competitive in their business models, materials/products/production processes developments using online digital technologies.

Innovation hubs are based on state of the art cloud technologies (private and public) providing the infrastructure for online platforms, that are essentially like "virtual competence centres" or "virtual institutes" providing access to the latest knowledge, expertise and modelling advances across all domains. Such innovation hubs should also be connected to regional centres helping bringing and connecting all key players together to collate all expertise from all Europe into one vibrant hub.

Examples of such hubs are the emerging Materials Modelling Marketplaces as envisioned by the EMMC. They provide foundations for collating all materials modelling expertise and assets, such as programs (commercial and open) on open and closed (behind firewall) online hubs.

A key vision is to render the innovation hubs, including the materials modelling marketplaces as registries of **"industry commons"** related to materials modelling assets and cast them in multitude of services including consultation, infrastructure and software as a service (IaaS and SaaS, respectively) capabilities.

Moreover, modelling services and assets such as data repositories and characterisation data that can assist in validation and verification of modelling is an important asset.

The integration of materials data together with models (both data based and physics bases) as well as novel data science paradigms and making them available on innovation hubs will give better access to all stakeholders to the immense potential benefits of digital emerging paradigms and enable more efficient development and deployment of integrated computational materials engineering workflows thus boosting and accelerating the integration of advanced well proven materials modelling into the PLM and product/material R&D in companies.

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Objectives

The objectives of the session is to present an expose of available innovation hub related activities and discuss how to increase the access to materials modelling related expertise and assets in the "industry commons" sense to all stakeholders in Europe. More specifically the objectives are:

- Integration of data and information from many more sources to inform new materials and product development in the future.
- Faster development and validation and verification and certification of models, and modelling tools
- Combining Materials Characterisation (MC) and Materials Modelling (MM) with AI (and semantics!) to drive faster development and update of materials modelling.
- Curation of Digital workflows for deep and continuous integration of materials modelling into product development and manufacturing
- Interoperable repositories of material properties (calculated and measured)
- facilitate validation and verification of modelling
- enhance the development of modelling software tools

Background information and documents

- https://emmc.info/wp-content/uploads/2018/01/European-Materials-Modelling-vision-beyond-2020.pdf
- http://the-marketplace-project.eu
- http://vimmp.eu
- https://emmc.info

Discussion points and questions

- How to stimulate the participation of modellers, software owners, and companies in using modelling services on innovation hubs?
- How to supporting Open translation environments and other hubs in addition to the marketplaces: what is needed?
- How to guarantee a long-term research investments in the development of advanced models and workflows for materials simulations, verification and validation?
- How can innovation hubs better support and boost the development of electronic, atomistic, mesoscopic, and continuum models towards more predictive modelling with new capabilities?
- Strategies to join up the methods and models to use data from different scales and different granularities, i.e. model interoperability, or Coupling & Linking?
- Is there a need to have one dedicated modelling innovation hub and how to connect it with other thematic hubs (like, innovation hubs for photonics, steels, light materials, etc…? How important are licensing scheme and access rights to software tools and services?
- What benefits would modellers/software owners/companies gain by sharing modelling workflows) and expertise? What are the conditions for sharing if at all?
- If you are a company, how would you utilise such innovation hubs (e.g., the marketplaces)?

- Advantages for software owners resulting from the innovation hubs?
- Importance of interoperability and EMMO for modelling services and digitalisation of workflows?