Accelerating innovations in building envelope materials using orchestrated multiscale material modelling workflows

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Abstract

It is well established that nearly 70% of product innovation relates back to the development of new materials or to the combination of existing materials in a new fashion (1). In specific use cases multiscale materials modelling has proved to be able to significantly speed up this process. However, despite the great promises and early successes, its widespread adoption within industry remains constrained. Recent analyses pinpoint data management, interoperability, the integration of experimental and modelling data across various time and length scales, and the automation of workflows as pivotal enabling technologies for unleashing the full potential of multiscale material design (2, 3). In the context of the EU-funded project Iclimabuilt, we present an approach that seamlessly integrates a materials information management system (Granta MI) with a robust simulation orchestration platform (OptiSLang) to facilitate, to automate and to orchestrate multiscale materials modelling alongside multiple simulation tools (4, 5).

In this presentation, we explain first how experimental materials data are captured from pilot lines and harmonized in a single repository (iDMS for Iclimabuilt data management system), before to be used as inputs for multiscale simulations. Then, through an advanced end-to-end multiscale workflow (from atomistic to building scale), we showcase framework's key concepts and features, illustrating its efficacy in estimating architectured composite material behavior from micro- to macro-scale, in the case of an insulation panel design test case made of innovative concrete development. Finally, we discuss how such multiscale workflow can be implemented as a reference template into a use-friendly ICME software framework (5).

References

(1) Souza, F. Why Do I Need Multiscale Modelling?", NAFEMS 2018

(2) Liu, X et al. Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems, NASA Technical Report

(3) Adamovic, N et al. EMMC roadmap for Materials Modelling and Digitalisation of the Materials Sciences, 13/11/2020

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(4) https://iclimabuilt.eu/

(5) Di Stefano, D., Developing a Software Framework to Design and Optimize Materials (2023)