Minisymposium at ICIAM 2019, Valencia, 16th July 2019
"Molecular and Mesoscopic Modelling in Chemical Engineering Data Science"

Track: MIA.4 – "Industrial mathematics infrastructures around the world to promote industry-academia collaborations"

Organizers:
- Martin Horsch, STFC Daresbury Laboratory, UK, martin.horsch@stfc.ac.uk
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Minisymposium abstract

Reaching quantitative agreement with available experimental data, and predicting properties where data are absent, molecular and mesoscopic modelling transforms chemical engineering data science. This minisymposium discusses virtual marketplaces and platforms by which the knowledge from multiscale modelling and simulation can be transferred to engineering practice. This requires an institutionalized collaboration between academic and industrial engineering, scientific computing, and applied mathematics, and jointly governed semantic assets to ensure the interoperability of models, numerical solvers, and databases. Initiatives working toward this (FORCE,* MarketPlace,* and VIMMP*) are represented at the minisymposium jointly with *translators* who connect method development with engineering practice.

Participants and talks

Gianluca Boccardo, Antonio Buffo, and Daniele Marchisio, "*From molecules to process-scale: Facilitating multiscale simulations in virtual marketplaces*"
Peter Klein and Marcel Burgard, *"Formulations and computational engineering: The FORCE project approach"*
Arpit Singhal and Adham Hashibon, *"Building a marketplace for materials modelling services: Interoperable, integrated multiscale platforms"*
Martin Horsch, Silvia Chiacchiera, Michael Seaton, and Ilian Todorov, *"Reliable and interoperable computational molecular engineering"*
Graziano Frungieri, Gianluca Boccardo, and Marco Vanni, *"Multiscale simulations of industrial problems in an open simulation platform: The compounding of rubber materials as a case study"*
Patrice Malfreyt, *"Multiscale modelling of polymer materials: Recent advances and challenges"*

Schedule

Session I *(platforms)*, chair: M. Horsch

(1) 14:30 – 15:00 G. Boccardo
(2) 15:00 – 15:30 P. Klein
(3) 15:30 – 16:00 A. Singhal

Session II *(translators)*, chair: G. Boccardo

(4) 17:00 – 17:30 M. Horsch
(5) 17:30 – 18:00 G. Frungieri
(6) 18:00 – 18:30 P. Malfreyt

Contribution no. 1

From molecules to process-scale: Facilitating multiscale simulations in virtual marketplaces

Gianluca Boccardo, Antonio Buffo, and Daniele Marchisio,
Department of Applied Science and Technology, Politecnico di Torino, Italy

The VIMMP project* (https://vimmp.eu/) has the objective of building a web-based marketplace based on an ontological framework, linking different manufacturing industry sectors with relevant materials modelling activities, with the purpose to facilitate communication between model developers and end-users. In this contribution, an example of an industrial application (food emulsions production) of this integration is shown, where multi-scale CFD simulations and innovative "simulation-on-the-loop" machine learning strategies are used to aid in parameter estimation and increasing simulation accuracy.

Contribution no. 2

Formulations and computational engineering: The FORCE project approach

Peter Klein and Marcel Burgard,
Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany

In FORCE,* we integrate materials modelling workflows into Multi-Criteria Optimization (MCO). We strive for making MCO methods and tools available as decision methodologies. To this end, we develop a platform on top of an interoperable materials modelling suite to model Key Performance Indicators, used as MCO objectives, and to identify balanced compromises among them, the so called Pareto front. Decision making is supported by interactive graphical tools for the exploration of what-if-scenarios.

Contribution no. 3

Building a marketplace for materials modelling services: Interoperable, integrated multiscale platforms

Arpit Singhal and Adham Hashibon,
Fraunhofer Institute for Mechanics of Materials (IWM), Freiburg, Germany

The MarketPlace project* (https://www.the-marketplace-project.eu/) aims at developing an advanced semantic collaboration platform based on ontology that facilitates the integration of all materials modelling related services including databases of material properties, modelling workflows and translation of industrial problems into simulations and knowledge exchange. In this presentation, recent advances of the MarketPlace are demonstrated including novel services, Open Simulation Platform (OSP) approaches and standard wrapper design for interoperability between different materials modelling services on MarketPlace.

***Disclaimer concerning contribution 2:** FORCE is an EU funded Research and Innovation Action, Grant Agreement No. 721027, under topic NMBP-23-2016: Advancing the integration of Materials Modelling in Business Processes to enhance effective industrial decision making and increase competitiveness.

Contribution no. 4

Reliable and interoperable computational molecular engineering

Martin Thomas Horsch, Silvia Chiacchiera, Michael A. Seaton, and Ilian T. Todorov,
STFC Daresbury Laboratory, United Kingdom

To facilitate the advance of computational molecular engineering in process engineering data technology, community-governed standards need to be established to ensure the interoperability of models, numerical solvers, and databases. The present contribution reviews ongoing work on repositories, such as the MolMod database, semantic assets based on EMMO and MODA, and the potential of multicriteria optimization to allow industrial engineers to compute material properties reliably, with a characterized uncertainty, using bespoke molecular models; disclaimer on the VIMMP project,* see below.

Contribution no. 5

Multiscale simulations of industrial problems in an open simulation platform: The compounding of rubber materials as a case study

Graziano Frungieri, Gianluca Boccardo, and Marco Vanni,
Department of Applied Science and Technology, Politecnico di Torino, Italy

The development of Open Simulation Platforms (OSP) is a fundamental step towards further integration between model developers and end-users, facilitating the translation of real problems in a multi-scale simulation workflow. In the VIMMP project* (https://vimmp.eu/) the open-source code SALOME is used as an OSP. In this contribution, a real-world industrial case is studied using Code_Saturne (a CFD code integrated in SALOME) and an in-house Discrete Element Method code to investigate the compounding step of a rubber composite.

Contribution no. 6

Multiscale modelling of polymer materials: Recent advances and challenges

Patrice Malfreyt,
Université Clermont Auvergne and SimatLab, Clermont-Ferrand, France

Modelling of matter at a higher scale than the atomic scale raises many issues about how to develop coarse-grained (CG) models at this scale. Many generic CG models have been successfully applied to reproduce universal properties of polymer materials, but they are unable to account for the chemical nature of monomers. We propose to show how to develop realistic CG models that are capable of reproducing properties of interest for the industry.

***Disclaimer concerning contributions 1, 4, and 5:** The Virtual Materials Marketplace (VIMMP) project is funded within the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760907.

***Disclaimer concerning contribution 3:** The MarketPlace project is funded within the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760173.