14th World Congress on Computational Mechanics (WCCM XIV)
8th European Congress on Computational Methods in Applied Science and Engineering (ECCOMAS 2020)
*July 19- 24, 2020, Paris, France*

# INTEGRATION OF DISCRETE AND CONTINUUM/PROCESS MODELS FOR MATERIAL NANOTECHNOLOGY

## 1100 (ATOMISTIC, NANO AND MICRO MECHANICS OF MATERIALS)

**DR. E. LAURINI[+], DR. D. MARSON[+], DR. P. DE LUCA[*], PROF. P. ASINARI[#] AND PROF. S. PRICL[+]**

[+]MolBNL@UniTS – Dept. of Engineering and Architecture (DEA) – University of Trieste
Piazzale Europa 1, 34127 Trieste – Italy
erik.laurini@dia.units.it / sabrina.pricl@dia.units.it
www.units.it

*ESI Group
25, Rue Marcel Issartier, 33700 Mérignac – France
patrick.de.luca@esi-group.com
www.esi-group.com

[#]Multi-scale Modeling Lab – SmaLL - Department of Energy - Politecnico di Torino
Corso Duca degli Abruzzi 24, 10129 Torino – Italy
pietro.asinari@polito.it
https://areeweb.polito.it/ricerca/small/

**Key words:** Multi-scale Material Modeling, Process Modeling, Models Integration, Interoperabiliy.

## ABSTRACT

Scope description: This mini-symposium focus on the integration of the discrete computational methods at electronic/atomistic/mesoscopic scales with continuum/process/performance models for the description and the properties prediction of new nanomaterials of industrial interest. In particular, the topics could regard (i) the development of high-fidelity models to predict properties and behaviours of new nanomaterials at different scales – from quantum mechanics all the way up to process and performance simulations – (ii) the development of multiscale modeling pipelines that integrate these models across the scales, and (iii) the development of reference standards and standardized methods for the representation, storage, and communication of models and data.

Materials science and engineering is a field that has probably benefited most by the introduction of nanotechnologies, whilst the chemical industry is somewhat lagging behind. Likely, the lack of integrating the different specialized areas, both in terms of knowledge and computational tools, currently represents a formidable hurdle for these big industrial players.

Traditionally, industry has relied on continuum modelling at the macroscale. This can be attributed to the ability of these models to provide a description of systems on device-relevant

scales. However, time has shown that these methods fail to capture the so-called nano-effect if the properties of nanomaterials at molecular level are not properly integrated in to macroscopic modeling. By addressing these scientific and technological limitations, the pivotal mission of the computational sciences in nanotechnologies is to open the access to multi-model and multi-field material and process modelling and simulation tools to the industrial world.

The ambition of this mini-symposium is to cover the more relevant aspects which are critical to the widespread adoption of multiscale material and process modelling techniques in industry academia.

Contributions to (i) state-of-the-art modelling techniques and guidelines for further model developments; (ii) interoperability requirements, frameworks and pipelines for linking models and software; and (iii) evaluation of the economic impact of materials modelling on industrial innovation are welcome.

You are encouraged to submit abstracts on these topics.