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COMPUTATIONAL TECHNIQUES FOR NANOCOMPOSITE AND NANOSTRUCTURED MATERIALS MODELING

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ABSTRACT

The main characteristic of nanocomposites is the so-called size effect, i.e. the impact of nanoparticle size on the effective properties and behavior, at fixed volume fraction. This size effect, which originates from phenomena located at nanoscale, is generally attributed to the high ratio of interfacial area to bulk volume. Accurately capturing this size effect remains a challenging task to address the issue of modeling nanocomposites or nanostructured materials.

Numerous studies address nanocomposite or nanoporous materials' size-dependent effective elastic properties, mainly relying on molecular dynamic simulations or numerical/analytical homogenization techniques incorporating the Gurtin-Murdoch surface elasticity theory. Moreover, in some recent publications, nonlinear behavior (plasticity, damage,…) of nanocomposite and nanoporous materials have been investigated.

Despite many aspects of common interest in molecular dynamics simulations and mean-field homogenization methods, there has been so far quite a limited interaction between the two fields. In the topic of "Atomistics, Nano and Micro-mechanics of Materials", this session aims at bringing together experts in both fields in view of promoting efficient ways of scales bridging.

All contributions to the session aim to equally cover recent advances in molecular dynamics, dislocation dynamics, mean-field and computational homogenization, phase-field approaches, etc. Contributions on mechanical aspects as well as on multi-physics coupling are welcome.