

Data driven computational strategies for bottom-up and top-down multiscale modelling

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Supported by the optimization solvers and recent advances in additive manufacturing (AM), tailored as-designed materials have gained much popularity and prominence in several industrial applications (robotic, bio-engineering, energy industry, building, ...). Their applications will be extended to different fields since they are of interest for the Industry 4G revolution. Accurate modeling in materials sciences and mechanical engineering needs bridging the different scales in order to suitably derive the predictive proprieties (bounds or estimates) using micromechanical based approaches and multiscale computational mechanics. Consequently, modeling structures with large volumes leads to big data structures with intractable simulations cost. Rapid and optimal modeling and design of advanced architected materials need to merge computational multiscale mechanics and data sciences tools. In this work we illustrate the high interest of integrating data driven strategies in two-scales computations for both upscaling and downscaling modelling. The first example deals with sequentially multiscale simulations based on surrogate models and data driven computational mechanics paradigm [1]. At the offline stage, a training step is carried out with full non-linear computations over the Representative Volume Element (RVE). The input parameters for this training step are the imposed macro-variables over the RVE as the microstructures parameters (morphology and material parameters), whereas the output quantities of interest are the local fields (temperatures, displacements, ...). Direct numerical simulations are run at this stage. Spatial averaging of these fields leads to a data basis of the macroscopic material behavior stored only as data information without any explicit mathematical law (*model-free* constitutive macro behavior). The material data set is then investigated for macro-computations using a data driven computational approach [2] based on the double distance minimization algorithm between the manifold of physical constraints (conservations laws and boundary conditions) and the material data manifold (macro data obtained from micro-computations). Once the macro-problem is solved, one can obtain local fields thanks to a reduced order based surrogate model [3]. The second example illustrates the investigation of data driven offline-online computational strategies in the top-down multiscale modeling for the inverse design of architected materials with prescribed effective properties. An application to two scales topology optimization of 3D structures with architected materials will be presented [4].

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