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# Data-driven simulations from multiphase material databases augmented by active learning

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## Abstract

To overcome well-known drawbacks of classical phenomenological constitutive modeling of complex heterogeneous materials, a popular approach is the so-called computational homogenization (CH). In this full-field homogenization tool, the spatial arrangement and constitutive behaviors of the constituents in a representative volume element (RVE) are finely described, in order to derive an average mechanical response. A popular computational implementation, called FE2, encompasses two-level finite element numerical models, which circumvent the macroscopic constitutive modeling process (Feyel, 1999). However it quickly leads to prohibitive computational costs, even for problems with a modest number of degrees of freedom. A popular strategy in the literature to alleviate such computational burden is to use machine learning-based surrogate constitutive models (Matouš et al., 2017; Peng et al., 2021; Su et al., 2022) but this clashes with the original intention of bypassing the need for a macroscopic constitutive model. Conversely, the so-called (model-free) data-driven computation mechanics (DDCM) paradigm (Kirchdoerfer & Ortiz, 2016) proposes the direct integration of "experimental data", completely bypassing the need for explicit constitutive laws. The main goal of this work is to show how the DDCM approach can be used in synergy with CH to avoid fully-coupled multi-scale computations. A naive approach to using multi-scale constitutive behavior along with DDCM is the offline construction of a database via CH by assuming some sampling of the strain-space (Karapiperis et al., 2020; Xu et al., 2020). This approach is limited since the region of the strain-space covered during a simulation is problem-dependent. Instead, in the present work, we propose to bridge DDCM and CH into a semi-supervised machine learning tool using the Active Learning (AL) framework. Following AL jargon, CH is considered as the *oracle* responsible for labeling data: it provides the label "homogenized stress" for a given strain. The objective of this work is then twofold: (i) to provide valuable evaluations of the strain worth labeling from a boosted DDCM algorithm to the CH oracle in order to (ii) build a material database on-the-fly from carefully selected microscopic evaluations. We show through meaningful numerical examples that the proposed framework results in significant computational savings if compared to standard FE2 (Rocha

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et al., 2024). In addition, we discuss the relevance of the computed data points and how "rich" a database should or can be to properly represent the macroscopic material behavior. References:

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