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Model-free Data-Driven Approaches for Multiscale Mechanics of Solids

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Abstract Model-free data-driven computational mechanics (DDCM) [1] allows to solve boundaryvalue problems (BVP) without recourse to explicit constitutive models, using instead point wise strainstress data (organized in histories when relevant). This paradigm can actually be extended to several other physical phenomena (diffusion, transport, electro-magnetics) which can be formulated through field theories. Among other benefits, this offers an interesting outcome to computational multiscale mechanics (and physics), where it is often a challenge to fit the complex effective response of heterogeneous microstructured materials to specific phenomenological models. Indeed, this allows to efficiently use generated data, without the hassle of explicit models parameter identification. Solving a BVP then amounts to minimizing the distance between a data set and manifolds of admissible strain and stress fields. Interpreted in the framework of Game Theory [2], this problem can be addressed by a collaborative strategy, leading to a mixed integer quadratic programming (MIQP) problem [3], or by an adversarial strategy, leading to a formulation closer to classical nonlinear FE solvers.

Different strategies can be adopted to generate data, for example from RVE computations. Data sets can be generated a priori (sometimes referred to as offline generation), by exploring various load cases (for example [4]). But this requires to have a prior idea of the loading scenarios for which the data will be used, hence limiting the efficiency of the approach. Alternatively, data can be systematically computed for each new load state explored in the BVP, leading to the FE² paradigm when FE is used at both scales. This latter approach is well known to be prohibitively computationally expensive, even considering high-end computer architectures.

The ideal solution thus appears to adapt the data set dynamically, sampling the space of mechanical states according to the specific problem at hand. Such strategy is analogous to the so-called active learning (AL), a class of semi-supervised learning algorithms where new labelled data are incorporated on-the-fly. The key issue lies on the decision criteria that drives the iterative process of dataset enrichment. DDCM being based on distances in this space, derivation of sampling criteria is relatively straightforward. Other criteria not exclusively relying on the DDCM distance, are also worth investigating, for example metrics used in the ML community. In history-dependent cases, distances can be measured on full histories, leading to a type of approach where simulations are repeated with successively improved data sets [5]. Some parallels with the reinforcement-learning (RL) techniques might be drawn in this context.

We will discuss these various approaches and illustrate their performances on some applications, ranging from non-linear elasticity [6] to elasto-plasticity [5].



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