IA for homogenization: prediction of morphological and mechanical properties of random heterogeneous microstructures

IA pour l'homogénisation : prédiction des propriétés morphologiques et mécaniques de microstructures aléatoires hétérogenèses.

ML approach to inverse homogenization

The theory of partial differential equations (PDEs) is the most privileged tool for describing the transport and mechanical properties of physical systems. In most situations of interest, the medium is heterogeneous (presence of porosity, cracks, reinforcements), and the problem cannot be dealt with homogenization theories alone [Milton, 2003]. The PDEs must then be solved numerically on a discretized domain, the prevailing methods being finite element techniques, based on a meshing of the domain [Reddy, 2019]. Alternatively, spectral methods (also known as “Fourier methods”) can be directly applied to an image of the heterogeneities, to estimate a medium’s effective and local response to a given sollicitation [Moulinec and Suquet, 1994]. Fourier-based numerical schemes are straightforward application of the theory of PDEs. By principle, they rely on an underlying Green operator for a fictitious homogeneous medium, which is the sought-for material’s effective response in homogenization theories. The convolution product involving the Green operator essentially decouples the source term and the material’s local response [Willot et al., 2014]. Recently, neural network frameworks have been developed that take advantage of this property to devise predictors for materials with varying domain shapes or sollicitations [Winovich et al., 2019]. The method relies on two representations in *latent spaces* for the source and local solution of the problem, obtained by training variational auto-encoders. Other methods relying on autoencoders and on variational formulations of the problem have been proposed [Tait & Damoulas, 2020]. For inverse homogenization problems, these methods offer a significant improvement compared to specialized neural network models focused on specific PDEs, which must be retrained for each new geometry [Weinan et al, 2017; Sirignano et al., 2018].

Deep-networks based on Green operators offer novel perspectives regarding, in particular, inverse homogenization problems, in which structures must be determined that satisfy certain imposed constraints, such as ones related to mass or compliance under given loads [Allaire, 2012]. One the one hand, the overall behavior of the material is driven by heterogeneities at a small length scale. On the other hand, it is difficult to assess which morphological criteria are sufficient for discriminating between the various possible material responses. Most linear homogenization theories (e.g. in elasticity) are notoriously restricted to one or two-point statistics [Hashin and Shtrikman, 1962], however, in principle, more narrow bounds on the effective response may be obtained using variational principles that include higher-order statistics [Beran, 1965]. In practice, however, these bounds become intractable beyond three-point statistics. In the present project we propose to use stochastic models and their characterization via the Choquet capacity [Molchanov, 2005] (restricted to point statistics or "spatial law") to determine physically-informed morphological criteria. Point statistics can be used to probe a material structures and essentially determines a random set (within certain certain classes of random sets). Additionally, we will use machine learning pipelines to infer physically-informed morpholgical criteria based on point statistics. Inversely, once such criteria have been identified, they can be used to tailor physical properties [Allaire et al., 2019]. It should homogenization bounds for non-linear problems also involve point statistics. Furthermore, extensions to *nonlinear* problems will be considered [Ponte Castañeda, 1992].

Main tasks and goals of the thesis

The project will be structured under two main tasks:
— *Deep-learning predictors for mechanical properties*. Various textures of porosity will be simulated using random sets (such as Boolean media, Boolean functions, Gaussian fields). A method based on variational autoencoders and Green operators projections will be used to predict the mechanical response of these materials under various loads.
— *Determination of mechanically-relevant point statistics.* Deep-learning pipelines will be constructed to match certain information, based on a medium's spatial law, with its mechanical overall response, determined in task 1. This method will then be combined with that of task 1 to perform inverse homogenization, in which structures will be classified according to their mechanical compliance and mass. Predictors for nonlinear problems (e.g. plasticity) will be investigated.

Thesis context

This thesis is proposed under a joint French-German PhD program, as a collaboration between *Mines Paris* and the *Fraunhofer ITWM/University of Kaiserslautern*. The PhD student will be jointly supervised by François Willot and Jesus Angulo (Mines) and Katja Schladitz (Fraunhofer) and work will be carried out in Fontainebleau, France (Mines Paris) and Kaiserslautern, Germany.

Candidates are advised to send a CV, cover letter and recent grades to F. Willot (francois.willot@mines-paristech.fr) and J. Angulo (jesus.angulo@mines-paristech.fr).

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