Physics-Informed Surrogate Model for Forward and Inverse Problems in 3D Polycrystalline Elastostatics

Lucas Monteiro Fernandes*[1], Samy Blusseau[2], Philipp Rieder[3], Matthias Neumann[4], Volker Schmidt[3], Henry Proudhon[1], and François Willot[5]

[1]Mines Paris - PSL (École nationale supérieure des mines de Paris) – Centre des Matériaux – France
[2]Mines Paris - PSL (École nationale supérieure des mines de Paris) – Centre de Morphologie Mathématique – France
[3]Universität Ulm - Ulm University [Ulm, Allemagne] – Germany
[4]Technische Universität Graz – Austria
[5]Mines Paris - PSL (École nationale supérieure des mines de Paris) – Centre de Morphologie Mathématique, Centre des Matériaux – France

Abstract

We develop a physics-informed neural network pipeline for explicitly solving linear elastic micromechanics in three dimensions, on heterogeneous media with periodic geometry. Our main application is a representative volume element of a polycrystalline material. Our approach combines a convolutional neural network with residual connections and non-learnable layers. The latter are introduced to enforce the fields admissibility and constitutive law in a way consistent with so-called Fast Fourier Transform (FFT) algorithms. More precisely, differential operators are discretized by finite differences in accordance with the Green operator used in FFT computations and treated as convolutions with fixed kernels. The deterministic relation between crystalline orientations and stiffness tensors is transferred to the network by a non-trainable layer. A loss function dependent on the divergence of the predicted stress field allows to update the network parameters without further supervision by ground truth fields. The neural network is trained on untextured synthetic polycrystals with periodic boundary conditions, realized from a stochastic 3D microstructure model based on random tessellations. Once trained, the network is able to predict the periodic part of the displacement field from the set of crystalline orientation field (represented as unit quaternions) of an artificial volume element. The proposed self-supervised pipeline is compared to a similar model trained with a data-driven loss function. Furthermore, we analyze the accuracy of the predictions of both models over microstructures larger than the ones used for training, as well as over polycrystals generated with different parameters of the stochastic 3D microstructure model. Finally, we show how the trained neural network can be employed to perform an optimization by gradient descent of the crystal orientations of a polycrystalline microstructure. In our optimization procedure, we minimize the local equivalent Von Mises stress field with an isotropy constraint on the overall mechanical response.

*Speaker