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Machine learning of evolving physics-based material models for fast and accurate concurrent multiscale modeling

Iuri B.C.M. Rocha[1], Pierre Kerfriden[2,3] and Frans P. van der Meer[1]

[1] Delft University of Technology, Faculty of Civil Engineering and Geosciences, P.O. Box 5048, 2600GA Delft, The Netherlands, *i.rocha@tudelft.nl, f.p.vandermeer@tudelft.nl*

[2] Centre des matériaux, Mines ParisTech, PSL University, 63-65 rue Henri-Auguste Desbrueres BP87, F-91003 Évry, France, *pierre.kerfriden@mines-paristech.fr*

[3] Cardiff University, School of Engineering, Queen's Buildings, The Parade, Cardiff, CF24 3AA, United Kingdom

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Concurrent multiscale (FE^2) frameworks relying on machine learning-based surrogate modeling have become increasingly popular over the last few years. The appeal of these approaches lies in substituting the original expensive lower-scale models embedded at every integration point of the higher-scale mesh by surrogate models that are cheap to compute but can still reproduce complex constitutive behavior accurately. By alleviating the main bottleneck associated with FE^2, such approximate frameworks effectively expand the applicability of the method to much a broader range of applications.

Among several different surrogate modeling techniques, Feedfoward Neural Networks (FNN) and Recurrent Neural Networks (RNN) are by far the most popular [1]. Being universal approximators, these models can approximate arbitrarily complex material behavior. Yet, training these surrogates often proves to be far from straightforward: purely data-driven models cannot provide meaningful predictions outside their training spaces, and for path-dependent materials this entails sampling from an essentially infinite-dimensional space of arbitrarily long strain paths.

In this work, we take a step back and attempt to reintroduce classical constitutive models into network-based surrogates. We start by defining a physics-based constitutive model at the higher scale. However, instead of calibrating the model *a priori* (e.g. with numerical homogenization), we instead increase its flexibility by letting its parameters evolve in time. This evolution is learned by casting the parameters as latent variables that evolve through a hidden dynamics model approximated by a deep neural network. The constitutive behavior is therefore given by a hybrid network composed of an FNN encoder and a material model decoder, with classical thermodynamic internal variables (e.g. plastic strains) accounting for path dependency. This physics-based memory and the constitutive assumptions of the original model allow the hybrid network to be trained with significantly less data than state-of-the-art RNNs and generalize better to unseen strain paths. Moreover, the additional flexibility allows the evolving surrogate to describe more complex behavior than the original material model.

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