# Accelerating concurrent multiscale mechanical simulations through physics-infused machine learning of evolving material models

Iuri Rocha[1], Pierre Kerfriden[2,3], Frans van der Meer[1]

[1] *Delft University of Technology, Faculty of Civil Engineering and Geosciences, P.O. Box 5048, 2600GA Delft, The Netherlands*

*E-mail: 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*

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

*E-mail: pierre.kerfriden@mines-paristech.fr*

*Keywords:* Concurrent multiscale ($FE^2$), Machine learning, Constitutive modeling

Accurate simulation of advanced materials often requires modeling material behavior across multiple spatial scales. A popular modeling strategy consists in defining a suitable higher-scale material model *a priori* and calibrating its parameters through homogenization of a limited number of micromechanical models. However, the lower-scale behavior to be homogenized is often so complex that defining an accurate pre-calibrated macroscale model becomes essentially impossible. Such scenario motivates the choice for a *concurrent multiscale Finite Element* ($FE^2$) approach in which the higher-scale constitutive behavior is directly upscaled from micromodels embedded at each macroscopic integration point without loss of generality. Yet, although powerful, concurrent multiscale models are still not widely applicable due to their extreme computational costs.

In the last few years, several strategies to alleviate the computational requirements of $FE^2$ have been proposed, many of which consisting in substituting the expensive micromodel computations by cheap surrogate model approximations. Among these, Feedforward Neural Networks (FNN) [1] and Recurrent Neural Networks (RNN) [2] have become by far the most popular approach. Neural Network surrogates provide fast predictions and can approximate arbitrarily complex material behavior. On the other hand, they are purely data-driven models and therefore cannot provide meaningful predictions for new inputs outside their training spaces. This limitation is especially problematic when approximating path-dependent materials whose behavior depends on their complete strain history: in this case, training entails sampling from an essentially infinite-dimensional space of arbitrarily long strain paths.

With this work, we propose an alternative approach that combines the main strengths from both machine learning and classical constitutive modeling. We start by defining a physics-based constitutive model at the macroscale, but instead of calibrating it based on a set of lower-scale observations we introduce additional flexibility by letting its parameters evolve in time. In order to learn this evolution, we cast the material parameters as latent variables evolving through hidden dynamics captured by a deep Neural Network. This combination of an FNN encoder and a material model decoder results in a hybrid network with physics-based memory (the internal variables of the decoder) which can be trained with significantly less data than state-of-the-art RNNs. We demonstrate the capabilities of the proposed approach with an extensive set of numerical tests.

[1] *Rocha, I.B.C.M., Van der Meer, F.P., Kerfriden, P. European Journal of Mechanics – A/Solids, Vol 82, 103995 (2020).*

[2] *Ghavamian, F., Simone, A. Computer Methods in Applied Mechanics and Engineering, Vol 357, 112594 (2019).*