

Efficient multiscale simulations of additively manufactured alloys: Toward a hybrid approach combining FE^2 and FE-NN

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Abstract: Metafor [1], our in-house nonlinear finite element software, is now capable of efficiently performing both 2D and 3D finite element squared (FE^2) [2] simulations, as illustrated in Fig. 1. This efficiency is achieved through several optimisations, including the parallelisation of microscale finite element analyses, the computation of macroscopic tangent moduli via static condensation of the microscale Representative Volume Element (RVE) using only two nodes in 2D or three nodes in 3D, and various numerical enhancements. However, despite these improvements, the inherent computational cost of FE^2 remains a significant challenge for multiscale simulations.

In recent years, neural networks (NNs) have gained popularity as surrogates for microscale simulations, giving rise to the FE-NN paradigm as an alternative to conventional FE^2 approaches. While this method enables significantly faster online computations, it entails high offline costs associated with data generation and model training. Moreover, the accuracy of NNs is inherently limited to their training data, posing challenges in path-dependent microstructures, where all possible loading paths must therefore be considered. These paths are often generated using stochastic methods, such as random-walk algorithms, making it difficult for users to obtain a clear understanding of the dataset. Additionally, the reliance on complex NN architectures, such as recurrent neural networks (RNNs), gated recurrent units (GRUs), or long short-term memory networks (LSTMs), further increases training costs.

To address these challenges, we propose a novel hybrid approach that combines the efficiency of FE-NN with the accuracy of FE^2 . Rather than relying solely on a complex NN architecture, a simpler model, such as a feedforward neural network, can be utilised. Trained on a well-defined dataset of path-dependent microscale simulations, this NN efficiently predicts responses for known loading scenarios at a fraction of the computational cost. When an unseen loading path is encountered, the code dynamically switches from the NN to a classical finite element analysis of the microstructure, thereby transitioning from FE-NN to FE^2 . Fig. 2 presents a preliminary proof of concept.

This transition occurs independently at each Gauss point of the macroscale, allowing the multiscale simulation to maintain overall efficiency while ensuring that the neural network operates within its trained range. As a result, most of the macroscale domain benefits from the NN's speed, while only critical regions transition to a classical finite element analysis when the NN lacks accuracy. This strategy provides an optimal balance between computational efficiency—both in offline and online phases—and numerical precision.

Furthermore, while optimising computational cost, this strategy also enables users to analyse the microstructural response in critical regions where the transition to classical finite element analysis has occurred, thereby providing deeper insights into the material's microscale behaviour.

Keywords: finite element squared, neural networks, multiscale simulations

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References

- [1] MN2L Uliège Non-Linear Computational Mechanics Laboratory. Metafor, an object-oriented finite element code for the simulation of solids submitted to large deformations, 2025. <http://metafor.ltas.ulg.ac.be/>.

- [2] M. G. D. Geers, V. G. Kouznetsova, and W. A. M. Brekelmans. *Computational homogenization*, volume 522 of *CISM International Centre for Mechanical Sciences*, page 327–394. Springer Vienna, Vienna, 2010.
- [3] Ling Wu and Ludovic Noels. Self-consistency reinforced minimal gated recurrent unit for surrogate modeling of history-dependent non-linear problems: Application to history-dependent homogenized response of heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering*, 424:116881, May 2024.

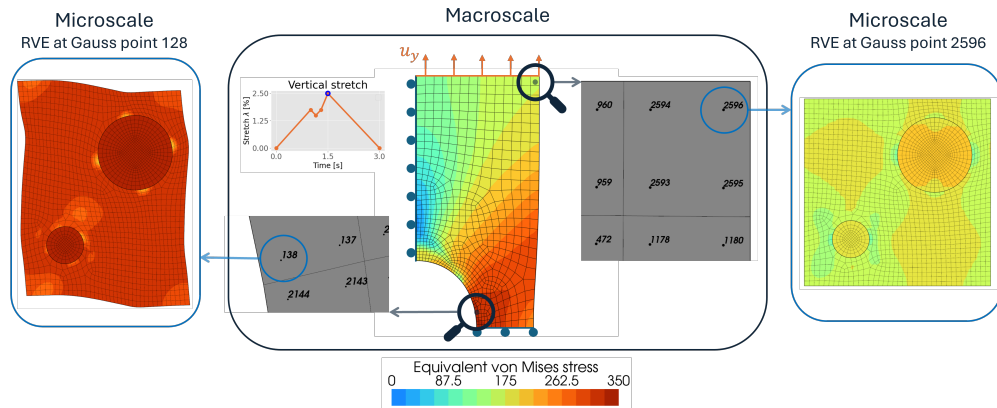


Figure 1: FE² simulation result from Metafor. This simulation is inspired by [3]. It includes 2,640 macro Gauss points and 116 computed steps, resulting in a total of 165 Newton-Raphson iterations. The RVE consists of elastic particles embedded in an elasto-plastic matrix. This Metafor FE² simulation took 1h50 on 64 cores, equivalent to 173 CPU-hours, and was 153 times faster than [3].

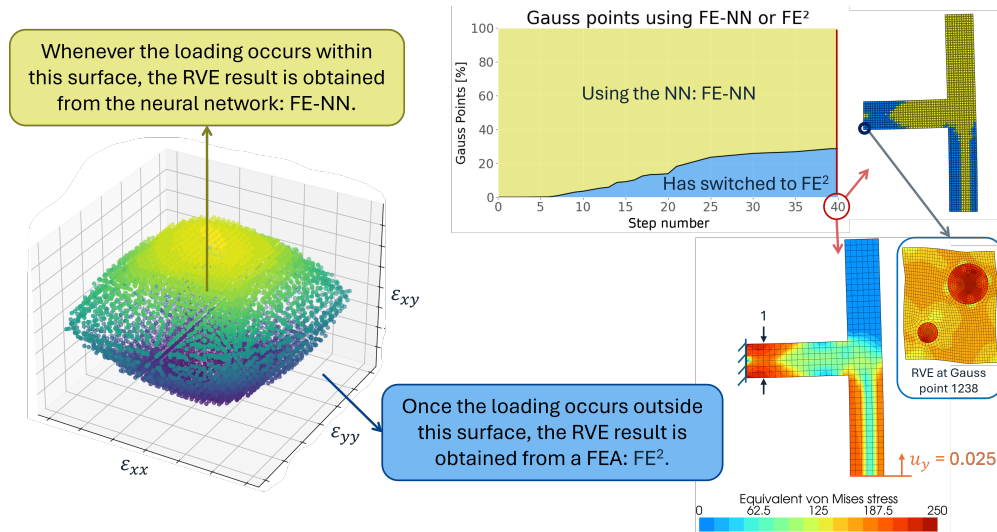


Figure 2: First proof of concept of the hybrid FE-NN and FE² method in Metafor. In this initial validation, the neural network emulates the elastic response of the RVE shown in Fig. 1.