Accelerating large-strain multiscale simulations through deep learning

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Context and objectives

Additive manufacturing (AM) is a key enabler in the space sector, particularly within the "New Space" or "Space 4.0" paradigm, which promotes satellite miniaturization, reusable launchers, and innovation. AM allows for groundbreaking structural designs that are **optimized and built as a single piece.**

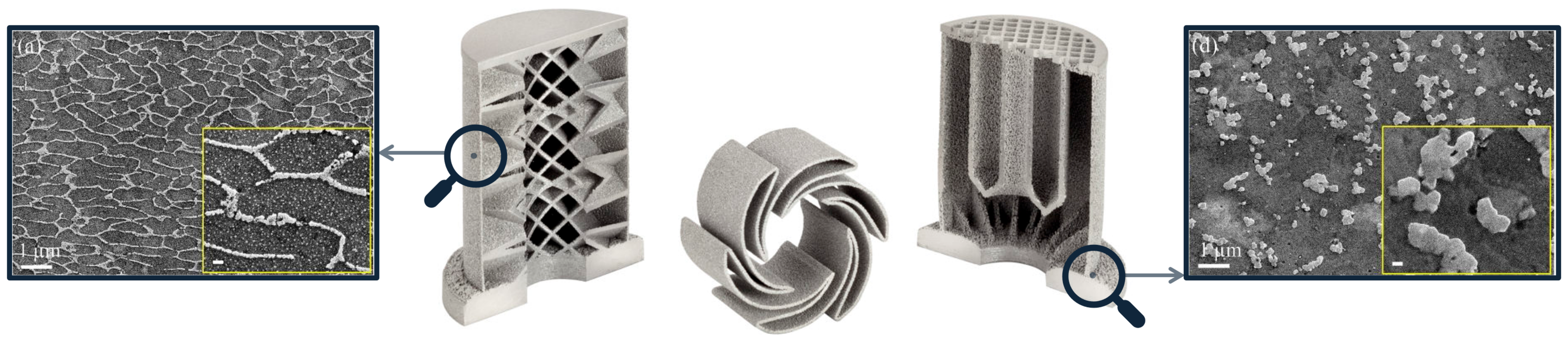

Figure 1. Two different 3D printed parts from mottcorp.com. Different microstructures of AlSi10Mg alloys obtained by additive manufacturing [1]: as built (a) and after stir friction processing (b).

- Meanwhile, new opportunities and challenges emerge from the **microstructure** resulting from AM processes and post-processing (e.g. gaps, porosities, inclusions, etc.), **affecting the material's strength and behaviors.**
- However, considering the microstructure with all its subtleties and potential effects on the macroscopic scale, **still remains a significant challenge.**
- While **multiscale methods** such as homogenization attempt to address these challenges, they remain **impractical for industrial applications due to their high computational cost.**

Hence, a key objective of this thesis is to **explore the potential of machine learning**, such as neural network surrogates, **for efficient multiscale simulations.**

All developments are implemented in Metafor [2], our in-house nonlinear finite element solver.

Why should we care about the microstructure?

- Traditional numerical methods often **overlook small-scale effects** or **assume homogeneity**, which does not reflect real-world materials. Multiscale analysis integrates microscale details, leading to **more accurate and realistic predictions.**
- Understanding the **link between microstructure and macroscale behavior** helps engineers optimize designs by considering how small-scale features influence overall performance.
- In additive manufacturing, numerical studies can help define **optimal microstructures** tailored for specific printing strategies.

- This is particularly **crucial for aeronautical and space structures**, where an optimized material representation enables **lighter and more efficient designs**, ultimately **reducing costs.**

FE² in our in-house nonlinear FEM code Metafor

Significant progress has been made in implementing an efficient parallel FE² [3] paradigm in Metafor.

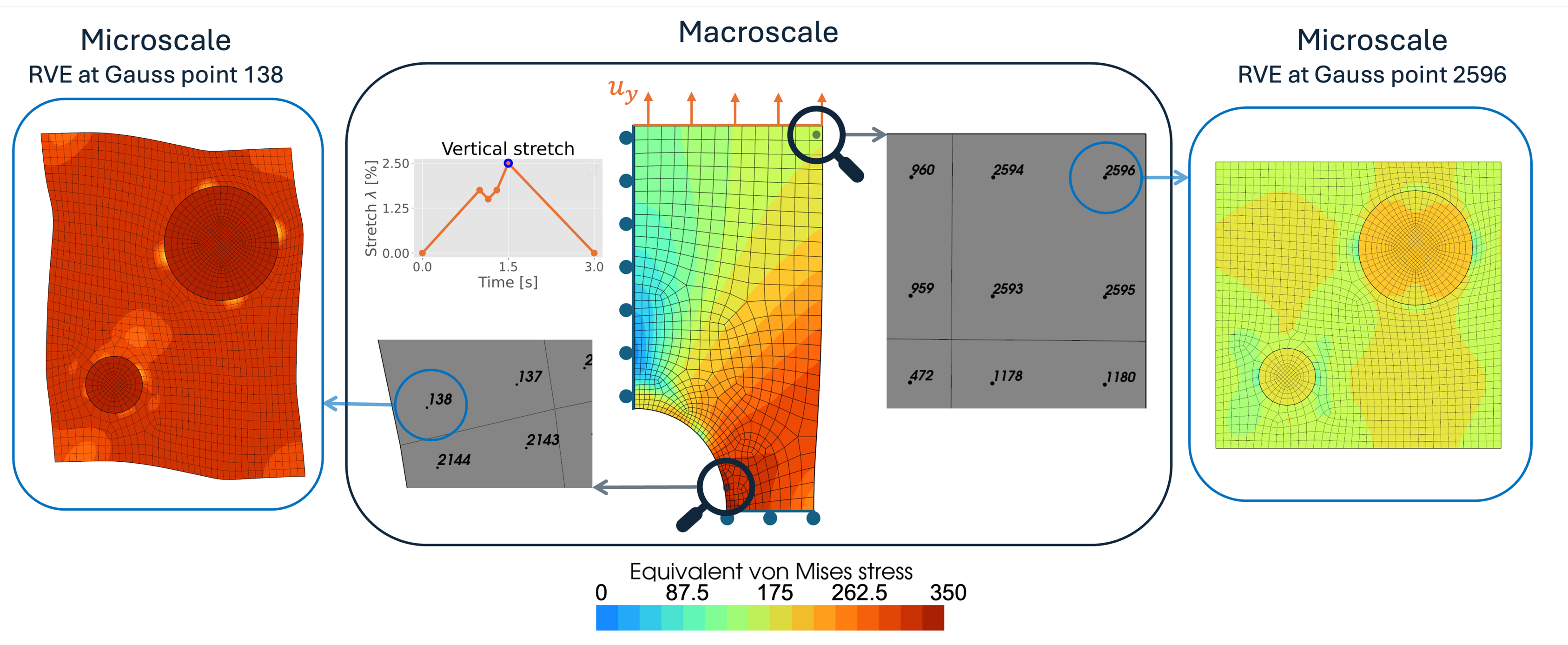

Figure 2. 2D plane strain FE² simulation using Metafor. The macroscale model consists of 700 linear quadrilateral elements, each with four integration points, while the microscale is discretized into 2,200 linear quadrilateral elements. The Representative Volume Element (RVE) features an elasto-plastic matrix with embedded elastic particles. **A total of 120 steps were computed, requiring 165 global iterations. The simulation was completed in 1h50 using 64 cores.**

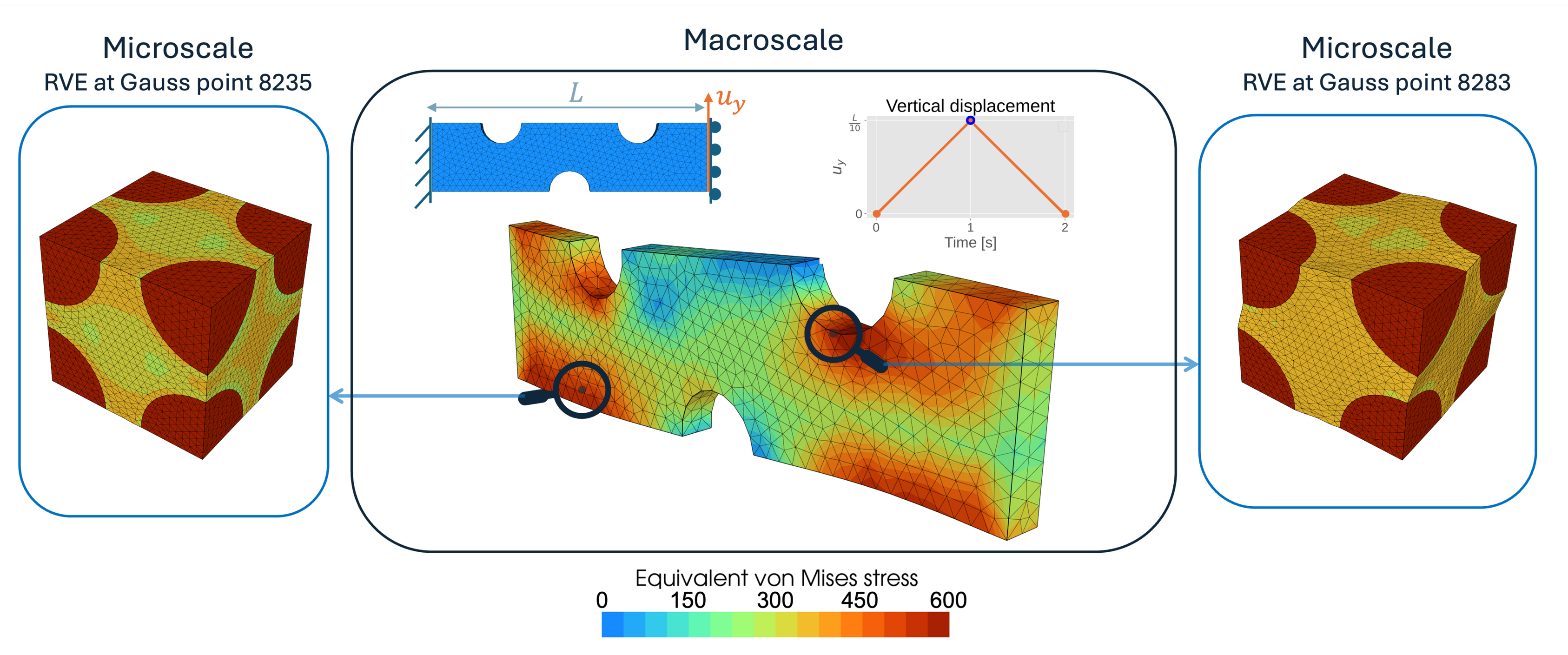

Figure 3. 3D FE² simulation using Metafor. The macroscale model consists of 4,470 linear tetrahedral elements, each with a single integration point, while the microscale is discretized into 43,000 linear tetrahedral elements. The RVE features an elasto-plastic matrix with embedded elastic particles. **A total of 75 steps were computed, requiring 127 global iterations. The simulation was completed in 47h20 using 64 cores.**

References

[1] Juan Guillermo Santos Macías. *Laser powder bed fusion AlSi10Mg damage and fatigue resistance improvement by post-processing.* PhD thesis, Université catholique de Louvain, 2021.

[2] MN2L Uliège Non-Linear Computational Mechanics Laboratory. Metafor, an object-oriented finite element code for the simulation of solids submitted to large deformations, 2024. `http://metafor.ltas.ulg.ac.be/`.

[3] 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.

Macroscopic stress & tangent modulus from the master nodes

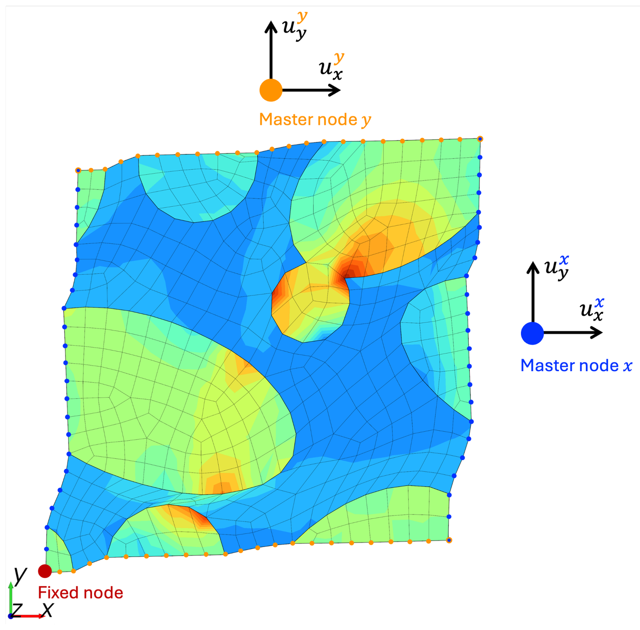

Figure 4. RVE with periodic domain, mesh, and highlighted master nodes.

Methodology:

- Periodic boundary conditions are imposed between opposite faces using Lagrange multipliers, driven by the displacements of the associated master node.
- From the macroscopic deformation gradient $\mathbf{F}$, displacements $\boldsymbol{u}$ are imposed on the two (2D) or three (3D) master nodes, driving the microscale boundary value problem.

The full macroscopic response can be extracted from the two (2D) or three (3D) master nodes:

1. The reaction forces $\boldsymbol{f}$ at the master nodes yield the macroscopic stress $\boldsymbol{\sigma}_{\mathrm{RVE}}$.
2. Static condensation of the RVE onto the master nodes yields the consistent macroscopic tangent modulus:

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{u}} \Rightarrow [\cdots] \Rightarrow \mathbb{M}.$$

Completely replacing the microscale model with a neural network?

A Neural Network (NN) can be viewed as a powerful function that has been rained to produce specific outputs given particular inputs by adjusting its internal parameters.

- ✓ "One could use such a tool to **accelerate multiscale simulations**, i.e., the neural network is trained using data from the microscale. In other words, the neural network **emulates the behaviour of the microstructure**. This approach is often referred to as FE-NN.
- ☞ While it does **reduce computation time** compared to vanilla FE², it is important to consider the **"offline resources" invested in generating the data and training the neural network.**
- ✗ Correct predictions only occur if the data—sets of inputs and outputs—have already been seen by the NN during its training. **Therefore, such an approach (FE-NN) must rely on large amounts of high-quality data.**

Toward a hybrid approach combining FE² & FE-NN

Instead, a simpler neural network, such as a feedforward neural network, can be used. Trained on a limited dataset of path-dependent microscale simulations, it efficiently handles known loading scenarios. **When the NN encounters an unseen loading path evolution, Metafor seamlessly switches from the NN to a finite element analysis of the microstructure, i.e. FE-NN → FE².** This process is performed independently at each Gauss point of the macroscale when needed.

In this proof of concept, a simple feed-forward neural network (FFNN) is used to model the elastic response of the RVE shown in Figure 3. The network has been trained to detect when input values fall outside the training domain, in which case its predictions are considered unreliable.

The offline phase required 30 minutes for data generation and 50 minutes for training on 10 cores. **Notably, this offline cost is amortised after just two simulations, as illustrated by the examples below.**

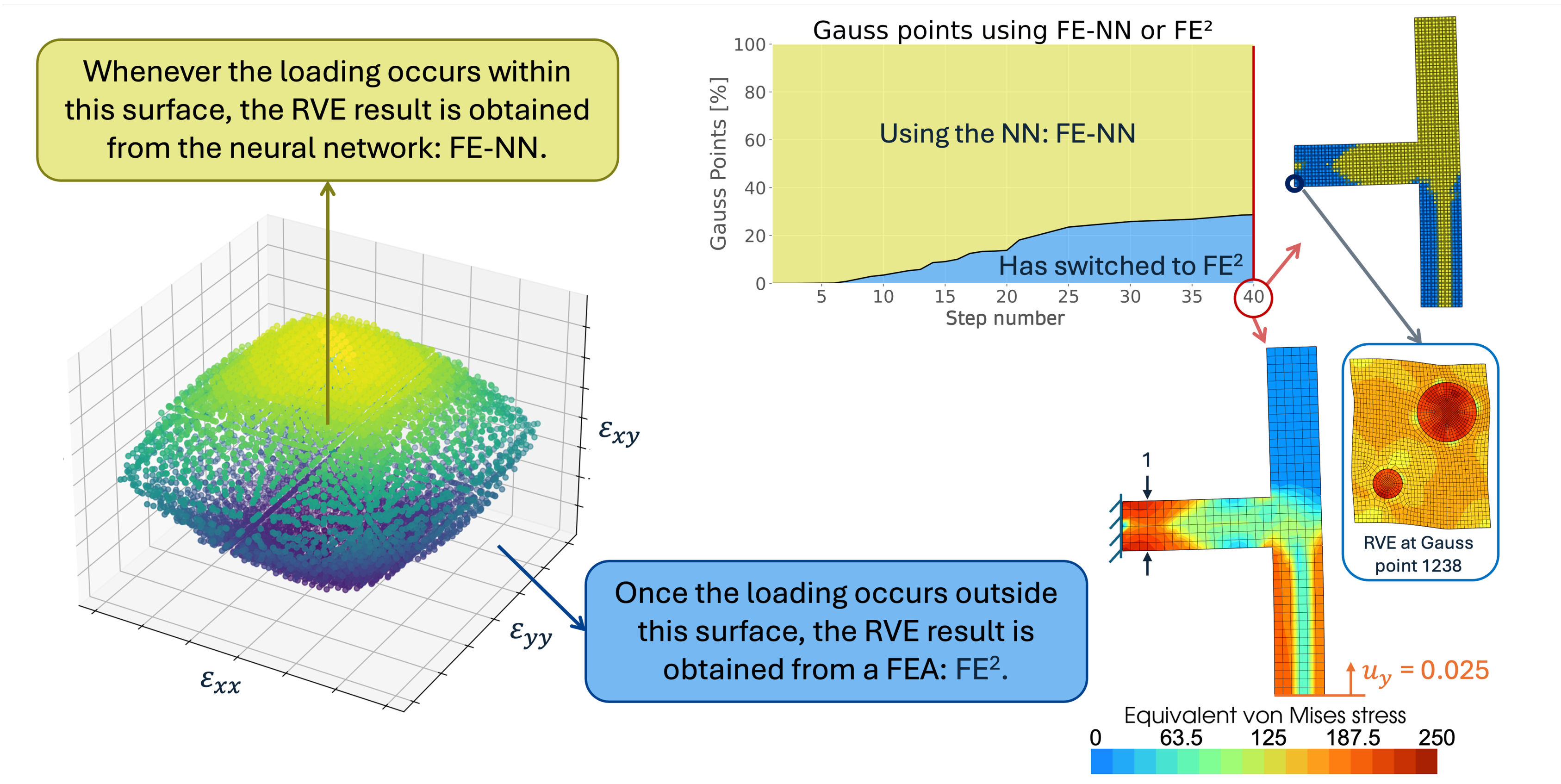

Figure 5. FE² simulation using Metafor with a hybrid approach. The macroscale model consists of 1,440 linear quadrilateral elements, each with four integration points. A total of 40 steps were computed. **The hybrid approach completed the simulation in 3 minutes, compared to 40 minutes for the classical approach on 10 cores. This resulted in a 12.3× speed-up in online computation time.**

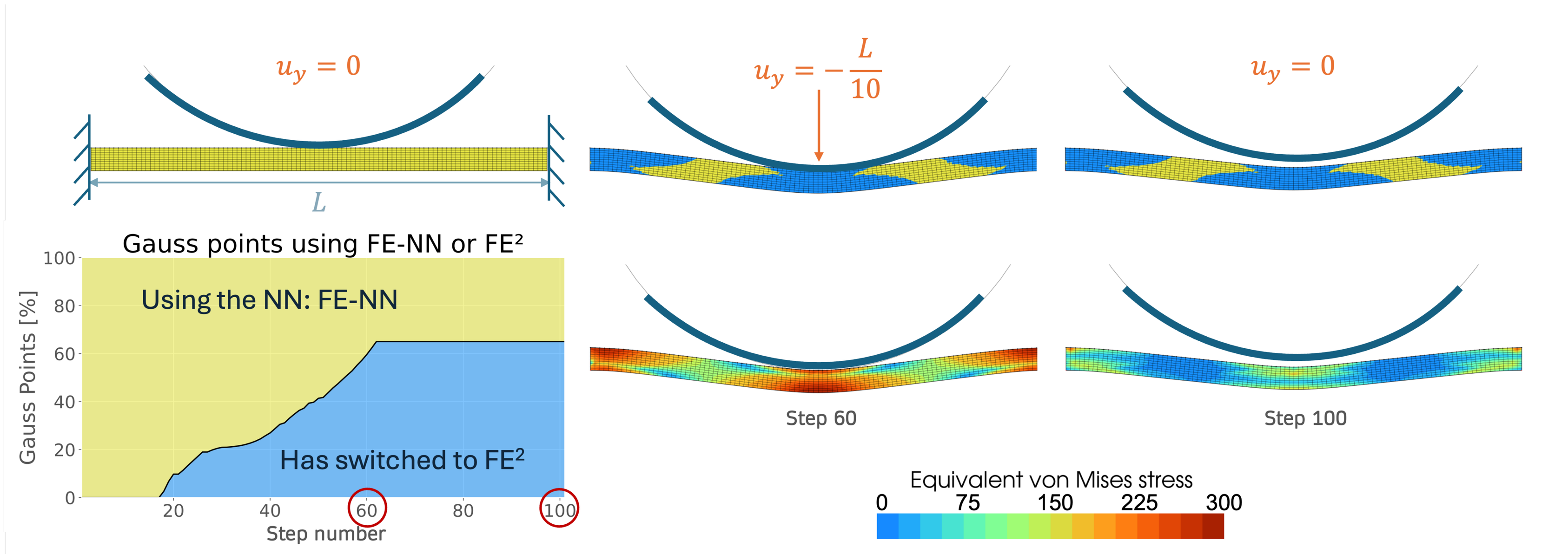

Figure 6. FE² simulation using Metafor with a hybrid approach. The macroscale model consists of 1000 linear quadrilateral elements, each with four integration points with four integration points. A total of 100 steps were computed. **The hybrid approach completed the simulation in 140 minutes, compared to 180 minutes for the classical approach on 10 cores. This resulted in a 1.3× speed-up in online computation time.**

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