

Context and objectives

Additive manufacturing (AM) is a key enabler for the space sector, supporting the “New Space” paradigm (miniaturization, reusable launchers, innovation). It enables optimised structures that can be **designed and manufactured as a single part**.

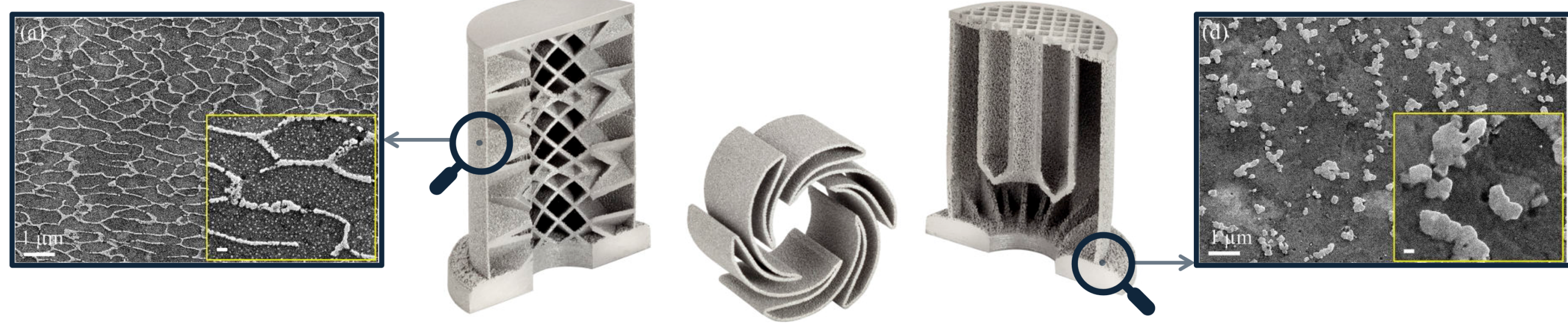


Figure 1. Microstructures of AlSi10Mg alloys: as-built (a) and after friction stir processing (b) [1].

- AM induces complex **microstructures** (porosity, inclusions, defects) that affect material behaviour.
- Capturing these effects at the macroscale remains a **major challenge**.
- **Classical multiscale methods** are accurate but **too computationally expensive** for industrial use.

Objective: develop fast and efficient multiscale simulations using machine learning (e.g. neural network surrogates) in Metafor [2], our in-house nonlinear FE solver.

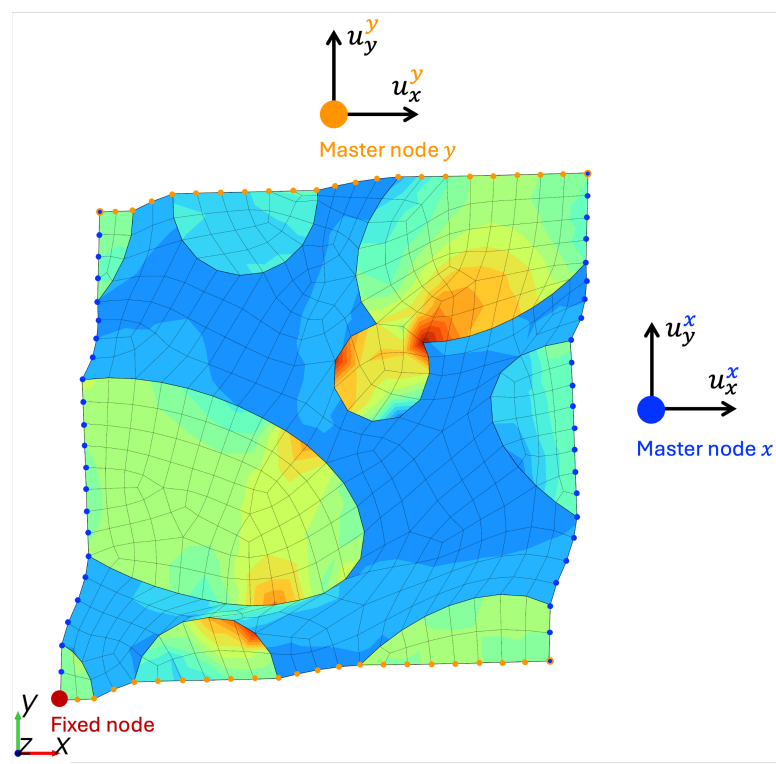
Why should we care about the microstructure?

- ✗ Traditional macroscale constitutive models **neglect microscale effects** or assume homogeneity.
- ✓ Multiscale approaches provide **more accurate and realistic predictions**.
- ✓ Understanding the **micro-macro link** enables better design and material optimisation.

Key impact: lighter, more efficient structures, leading to **cost reduction**.

Classical finite element squared

Principle: The constitutive response at each macroscopic Gauss point is obtained from a dedicated microscale FE simulation of a representative volume element (RVE) [3].



Methodology

- Macroscopic deformation gradient $\mathbf{F}$ drives displacements at master nodes.
- Periodic boundary conditions (Lagrange multipliers).

Key idea: homogenisation from the master nodes.

- Reaction forces $\mathbf{f} \Rightarrow$ macroscopic stress σ_{RVE} .
- Static condensation $\frac{\partial \mathbf{f}}{\partial \mathbf{u}} \Rightarrow$ macroscopic tangent modulus $\mathbf{M}$.

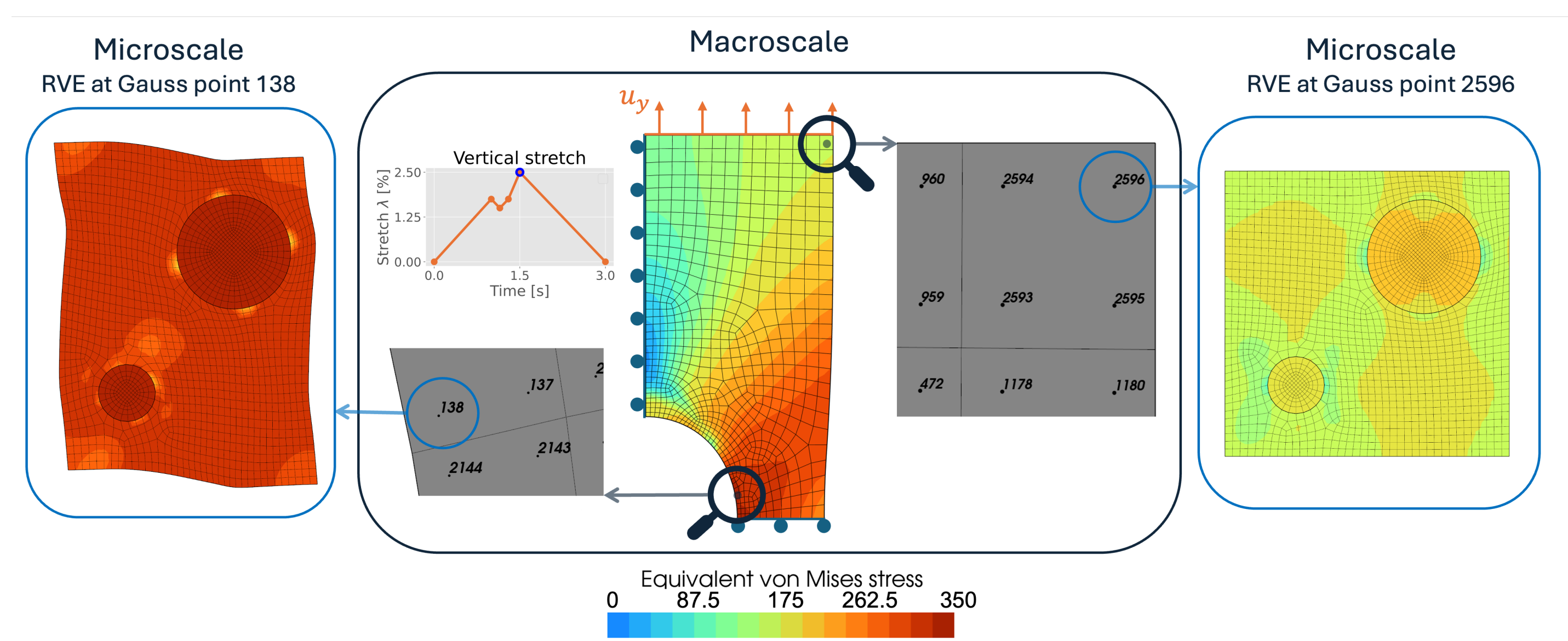


Figure 2. 2D plane strain FE² simulation in Metafor. Macro: 700 elements; micro (RVE): 2,200 elements (elastoplastic matrix with elastic particles). 120 steps, 165 iterations, 1 h 50 on 64 cores.

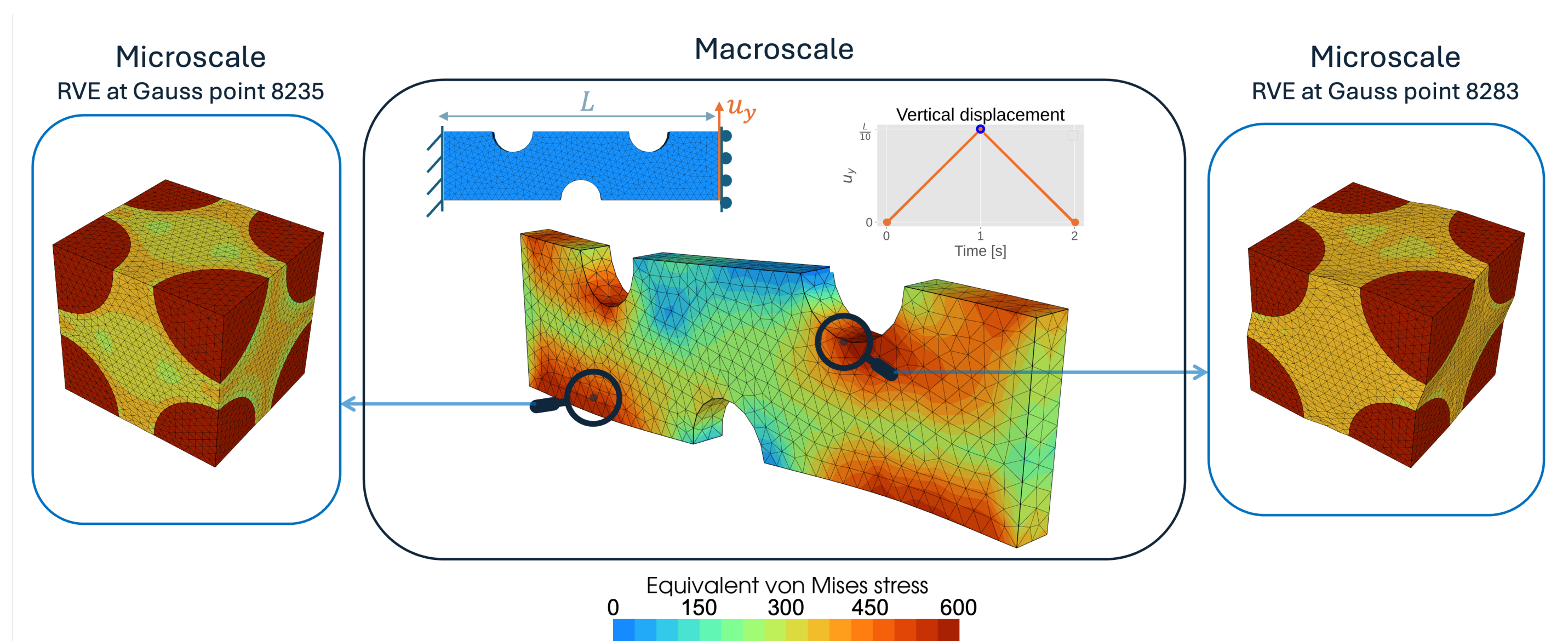


Figure 3. 3D plane FE² simulation in Metafor. Macro: 4,470 elements; micro (RVE): 43,000 elements (elastoplastic matrix with elastic particles). 75 steps, 127 iterations, 47 h 20 on 64 cores.

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 Uilège 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.ucl.ac.be/>.
- [3] R.J.M. Smit, W.A.M. Brekelmans, and H.E.H. Meijer, *Prediction of the mechanical behavior of nonlinear heterogeneous systems by multi-level finite element modeling*, *Computer Methods in Applied Mechanics and Engineering*, 155(1):181–192, 1998.

Stochastic finite element squared

Principle: The constitutive response at each macroscopic Gauss point is obtained from a microscale FE simulation of a representative volume element **randomly assigned to each macro Gauss point**.

Methodology: A set of $N = 16$ RVEs is generated from a stochastic distribution. At each macroscopic Gauss point, one RVE is randomly selected and used as its microscale FE simulation.

Key idea: Introduce spatial variability of the microstructure at the macroscale by assigning different RVEs, leading to a more realistic representation of the material behaviour.

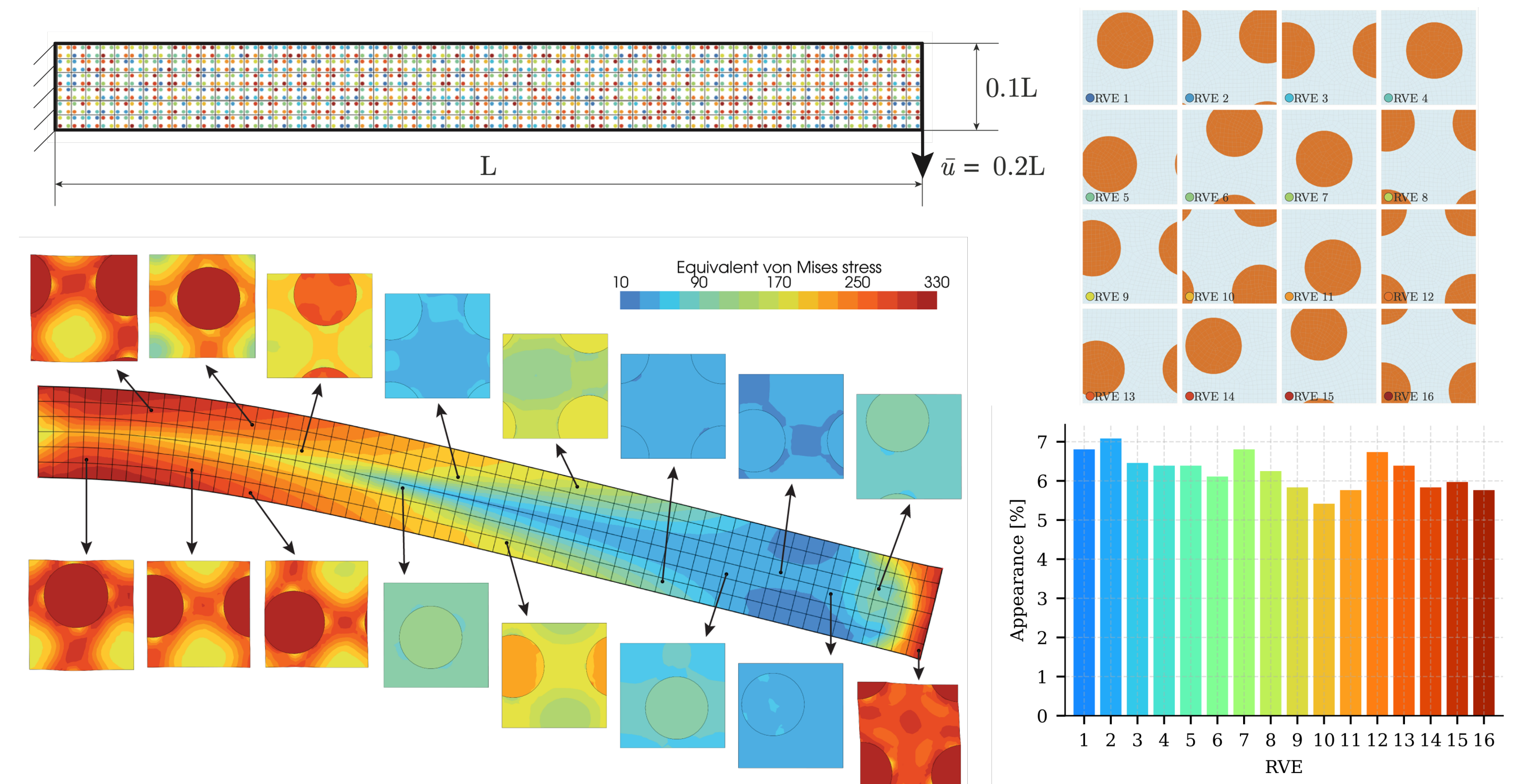


Figure 4. Stochastic FE² simulation in Metafor. Macro: 360 elements; micro: 16 distinct RVEs with, on average, 800 elements (elastoplastic matrix with embedded elastic particles). 28 steps, 53 iterations, 3 min on 32 cores.

Beyond two-scale simulations

Principle: Our methodology can be extended to three scales, i.e. FE³: macro, meso and micro. There are **266,240 micro FEA per macro iteration** and **361 million degrees of freedom** in total.

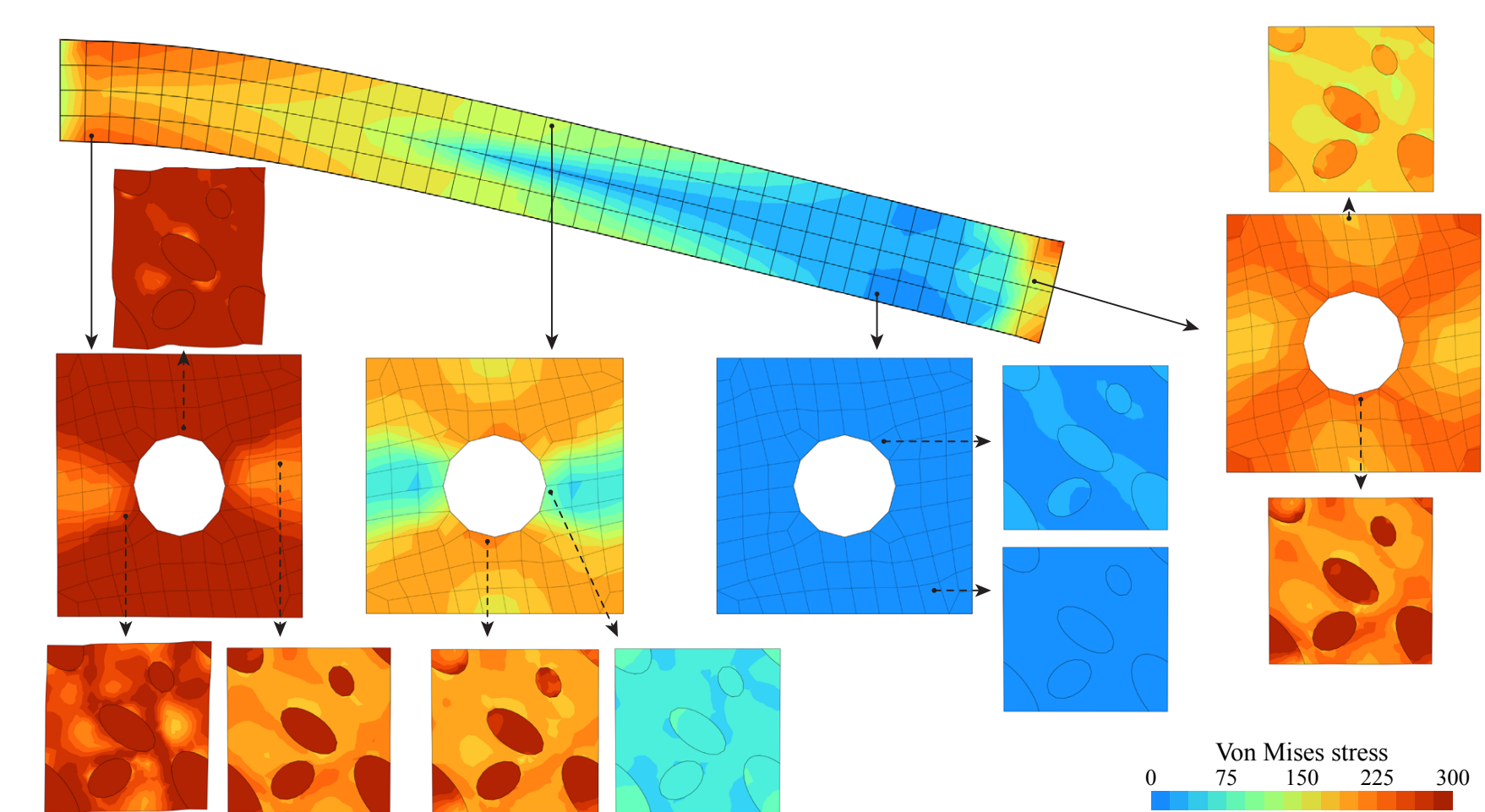


Figure 5. 2D plane strain FE³ simulation in Metafor. Macro: 40 elements; meso: 104 elements; micro 600 elements (elastoplastic matrix with elastic particles). 38 steps, 68 iterations, 3 days 11 hours on 32 cores.

Replacing the microscale model with a neural network?

A neural network (NN) is a powerful function trained to map inputs to outputs by learning from data.

- ✓ **Fast:** NNs can accelerate multiscale simulations by emulating microscale behaviour (FE-NN).
- ⚠ **Trade-off:** requires significant **offline cost** (data generation and training).
- ✗ **Limitation:** reliable only within the **training data domain** $\Rightarrow$ requires large, high-quality datasets.

Toward a hybrid approach combining FE² & FE-NN

Principle: NN for known loading paths (FE-NN), with an automatic switch to FE² for unseen or unreliable predictions, independently at each macroscopic Gauss point.

Methodology: Feedforward neural networks are trained to reproduce the elastic response of the RVEs.

Key idea: The NN detects when inputs fall into the plastic domain; in such cases, predictions are considered unreliable and a switch to FE² is triggered.

Offline cost: 10 min (data generation) + 10 min (training, 10 cores). **Amortised after a single simulation.**

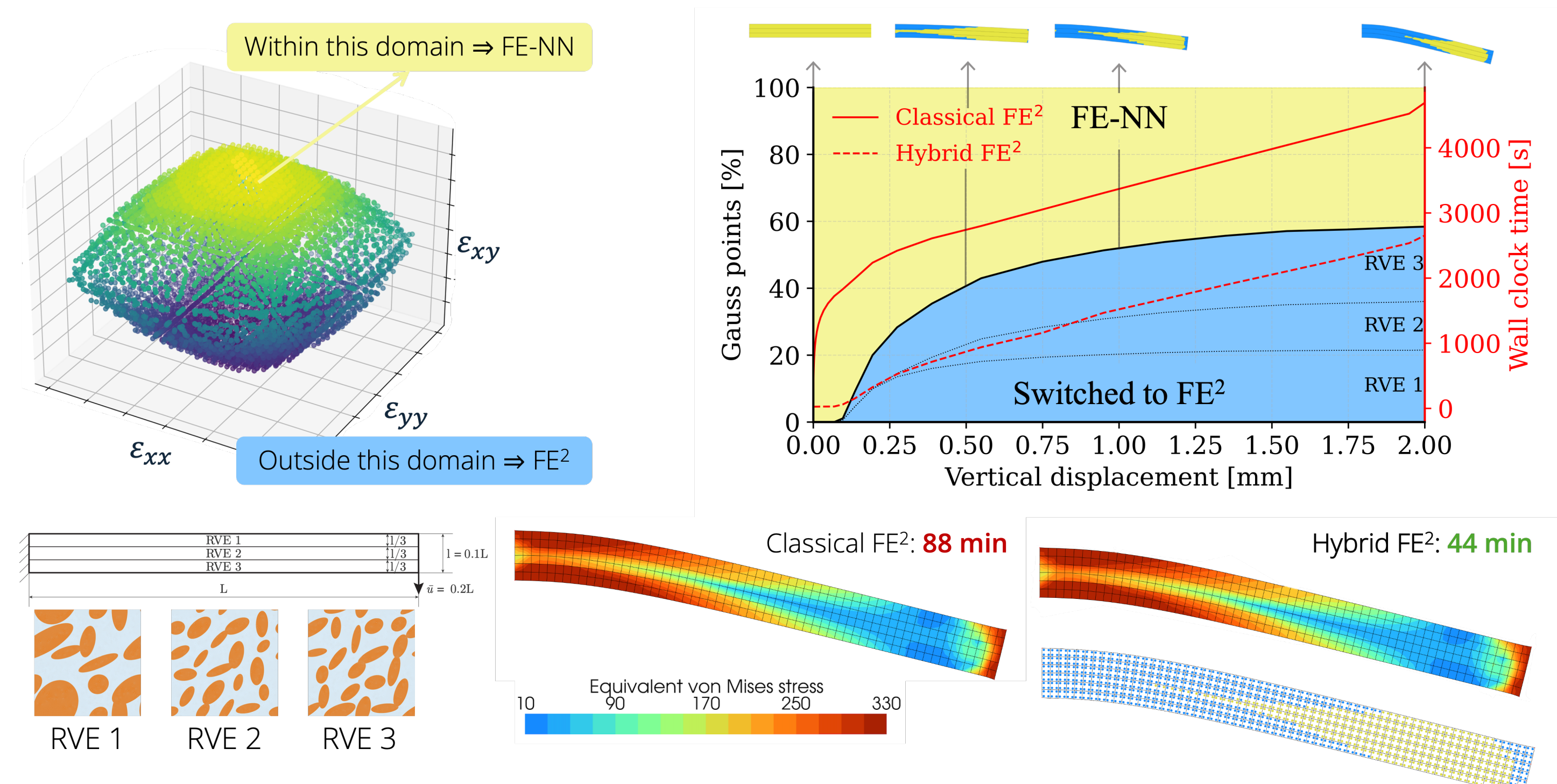


Figure 6. FE² simulations in Metafor with and without a hybrid approach. Macro: 360 elements; micro: three distinct microscapes, namely RVE 1, RVE 2, and RVE 3, discretised with 12000, 13000, and 13400 (elastoplastic matrix with elastic particles). 28 steps, 51 iterations, 1 h 28 (classical FE²) and 67 iterations, 44 min (hybrid FE²), both on 24 cores.

