Multiscale Thermomechanical Simulations of 3D Printed Materials using 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.

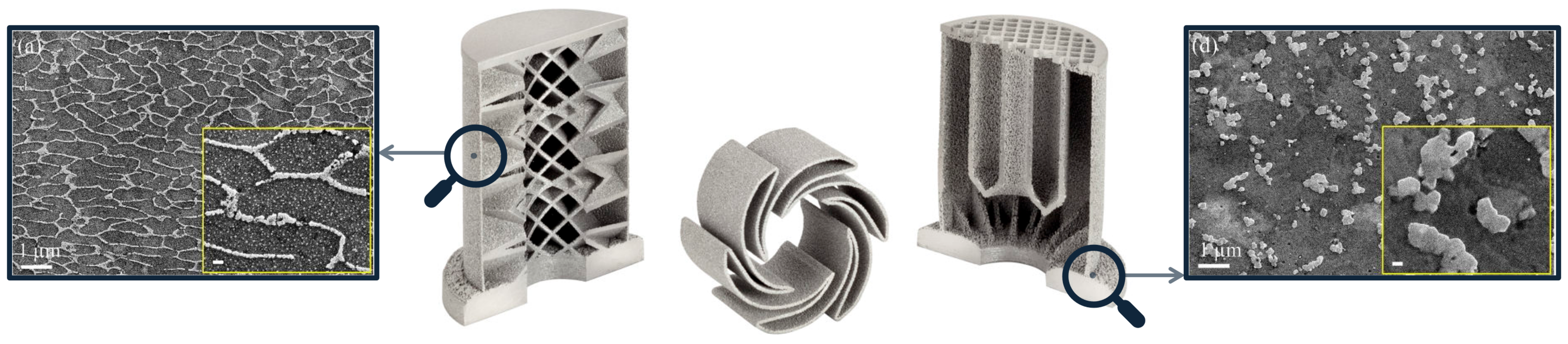

Figure 1. Two different 3D printed parts from mottcorp.com. Different microstructures of AlSi10Mg alloys obtained by additive manufacturing [1]: as built (a) and after stir friction processing (b).

- 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, especially in numerical simulations such as the finite element method.**

  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 for multiscale thermomechanical simulations. The goal is to substitute the microscopic scale with a neural network surrogate.

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

Non-linear finite element analysis

- Finite Element Method (FEM) is a numerical technique used to solve differential equations by dividing the domain into smaller, simpler sub-domains known as finite elements.
- The latter aims **to predict and analyze the behavior** of mechanical structures and components under different loading conditions to ensure **structural integrity** and **optimize design**.
- The **user must define** how the material responds to applied forces or deformation, i.e. choose the right **constitutive equations at macroscale**.

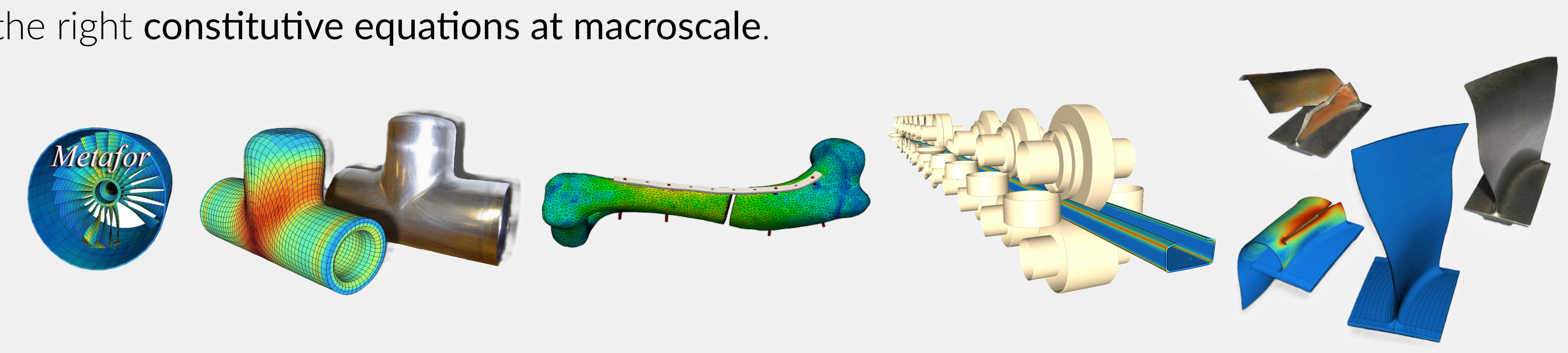

Figure 2. Examples of finite element analysis done with Metafor [2].

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**.

Multiscale analysis: the finite element squared (FE²)

- Taking into account **all length scales** in a conventional finite element analysis (FEA) is **unfeasible**. As always, there is the classical **trade-off between accuracy and computation cost**.
- This thesis is currently based on the finite element squared concept [3]:
  - Both **macro** and **micro** scales are **considered seperatly** in the FE simulation.
  - There is **no constitutive equation at the macroscale**; instead, the **behavior of the material** is obtained from a **representation of its microstructure (RVE)**.
  - Although the two scales seem separated, the **homogenization principle** manages the **scale transition**, i.e. the communication between them.

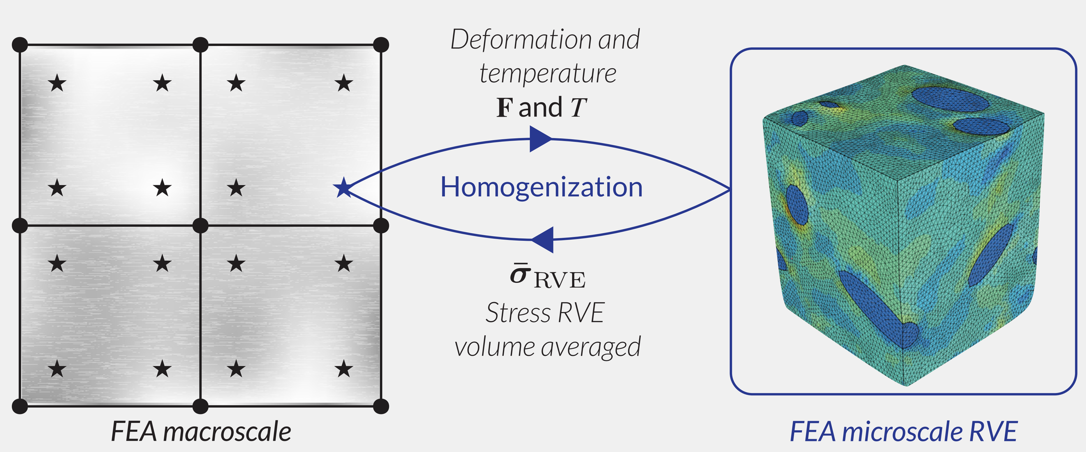

Figure 3. Finite element squared.

NEW: FE² in our in-house FEM code Metafor

Over the past year, **significant progress** has been made in implementing an efficient FE² paradigm in **Metafor**, with key features including:

- Large deformations.
- Parallelization at the macroscale, enabling multiple microscale FEA to be solved simultaneously.
- Material tangent moduli $\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}}$ can be obtained either through static condensation of the RVE FEA or numerical perturbation.
- Fully operational in 3D.

The FE² simulation presented below consists of 700 elements with four integration points at the macroscale and, 2200 elements at the microscale. The Representative Volume Element (RVE) consists of an elasto-plastic matrix with embedded elastic particles. **A total of 120 states were computed, requiring 165 iterations, which took 1h50 on 64 cores.**

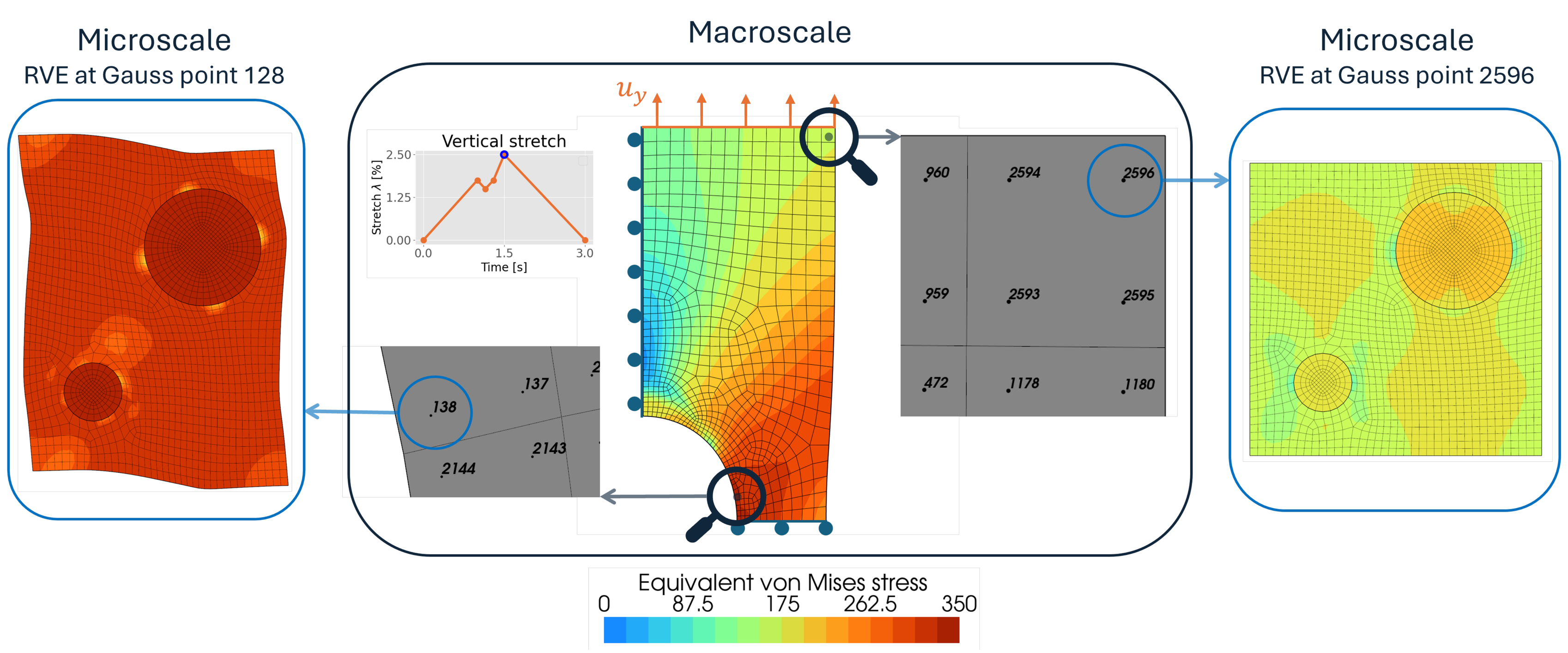

Figure 4. Finite element squared simulation from Metafor.

Replacing the microscale by a neural network

- A **neural network** (NN) can be viewed as a **powerful function** that has been **trained** to produce **specific outputs given particular inputs** by adjusting its internal parameters.
- **Correct predictions** only occur if the data—sets of inputs and outputs—have **already been seen by the NN during its training**. Therefore, neural networks rely on **large amounts of (quality) data**.

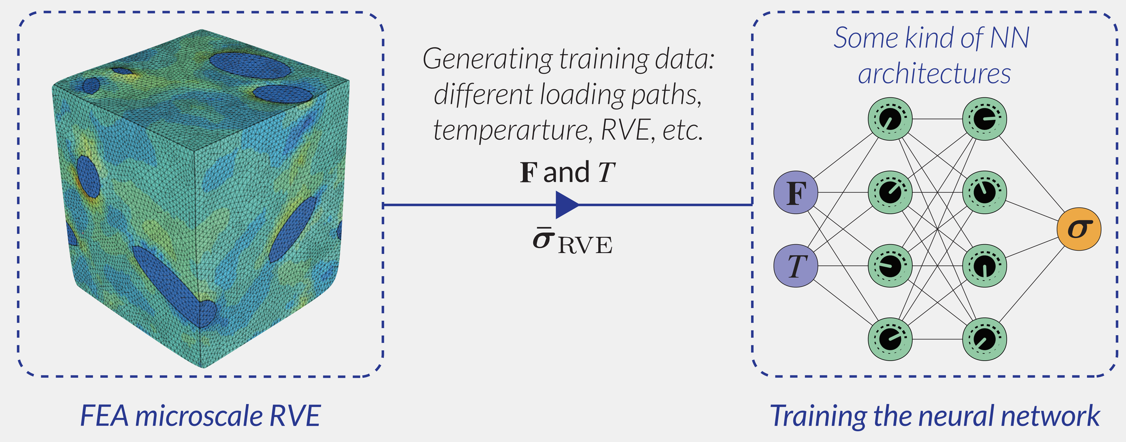

Figure 5. Training a neural network.

- One could use such a tool to **accelerate multiscale** simulations, i.e. the neural network has been trained with data from the microscale. In other words, the neural network **emulates the behavior of the microstructure**.
- 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.

NEW: 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.

The hybrid FE² simulation presented below includes 1440 elements with four integration points at the macroscale and 2200 elements at the microscale. A total of 40 states were computed. The hybrid approach completed the simulation in 40 min *(offline: 30 min for data generation and 50 min for training)*, compared to 140 min for the classical approach on 10 cores. In this proof of concept, the NN is used for the elastic part of the RVE from Figure 4. **This resulted in a 3.5× speed-up. Even accounting for the one-time training cost, the hybrid method remains more efficient than classical FE².**

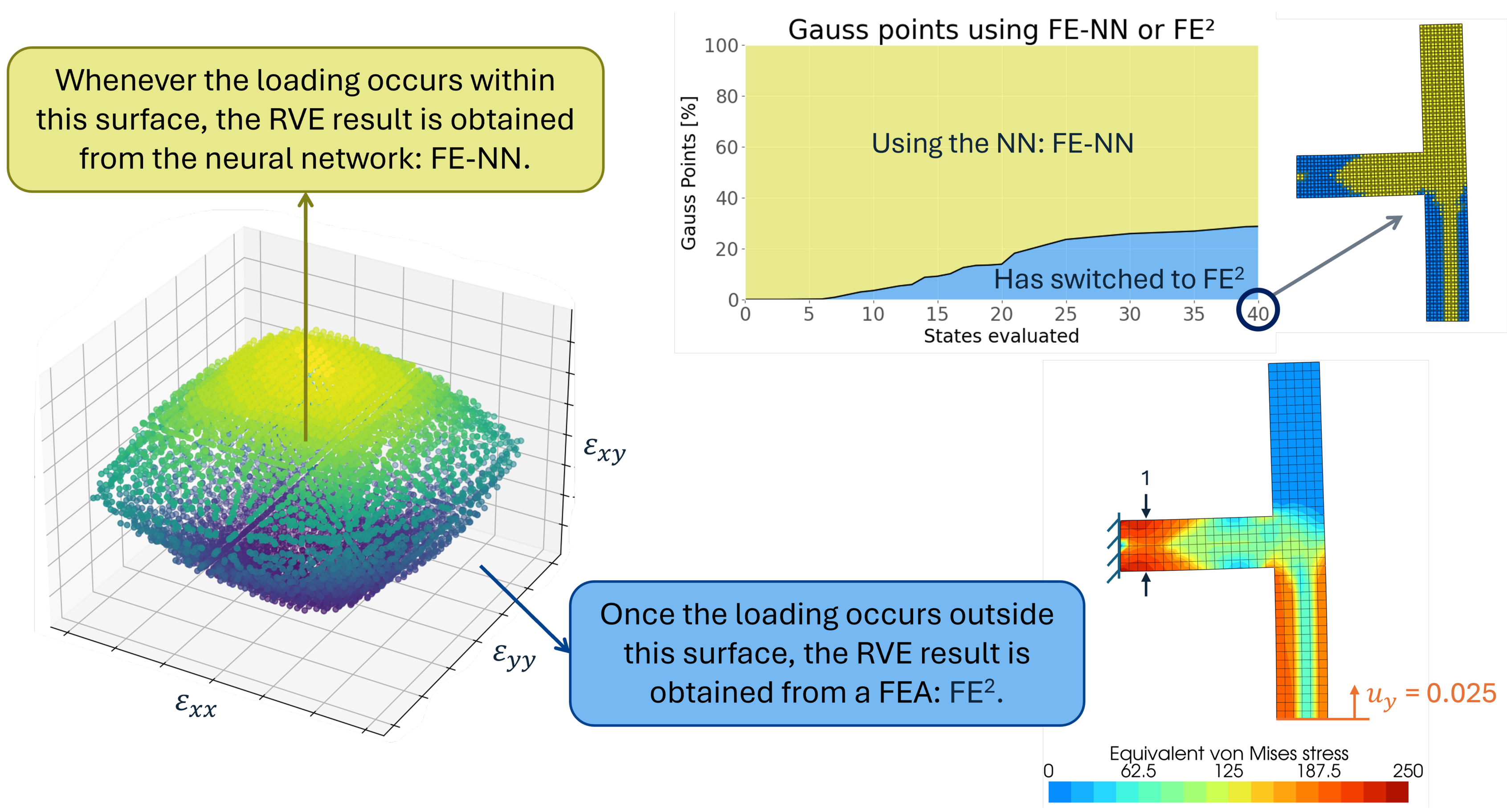

Figure 6. Finite element squared simulation from Metafor with a hybrid approach.

References

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Space4Relaunch

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