Multiscale Thermomechanical Simulations of 3D Printed Materials using Deep Learning

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Context

- Additive manufacturing holds significant potential in the space sector, especially within the context of the "New Space" or "Space 4.0" paradigm, which emphasizes novel satellite architectures and their miniaturization, reusable launchers, innovation, etc.
- In particular, AM enables innovative structural design, opening up new possibilities:
  - optimized and built in one piece;
  - unmanufacturable using conventional methods;
  - made off materials with intriguing properties, such as self-healing capabilities.

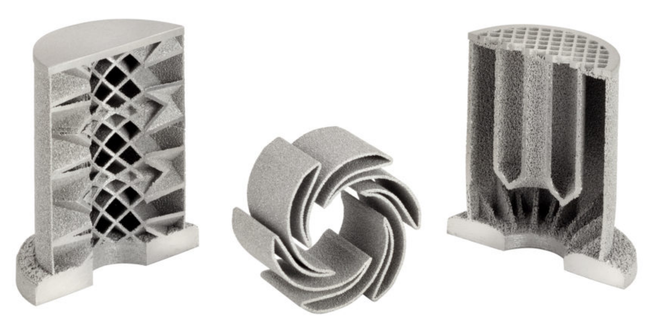
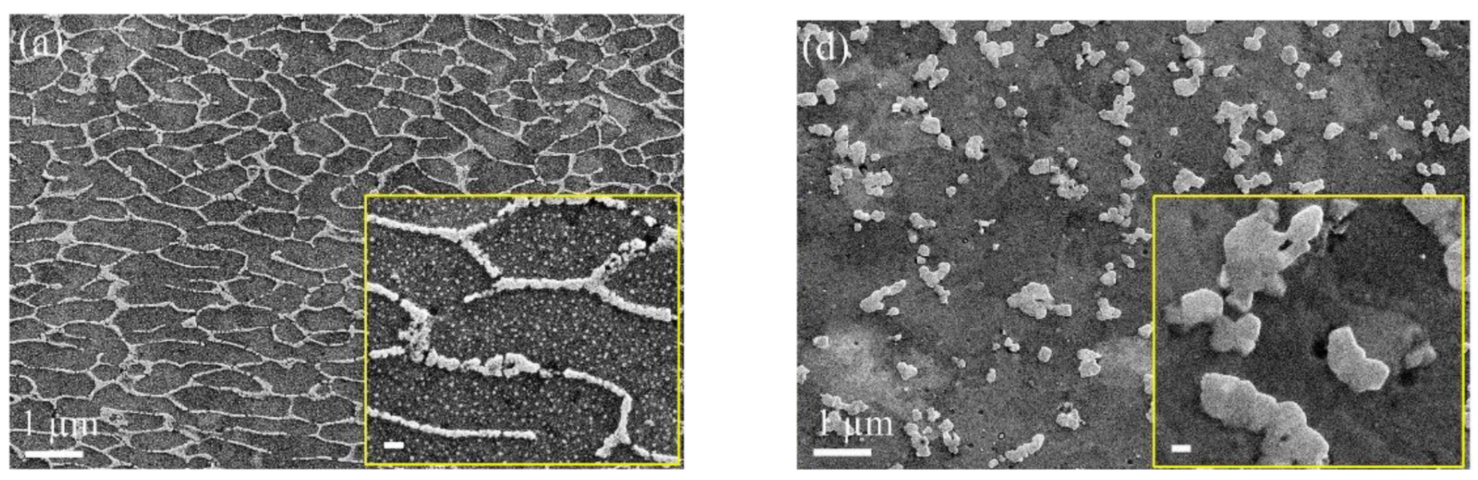


Figure 1. Two different 3D printed parts from mottcorp.com.

- 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**.



(a) As built. (b) After stir friction processing.
Figure 2. Different microstructures of AlSi10Mg alloys, obtained by additive manufacturing [1].

➤ However, taking into account the microstructure with all its subtleties and potential effects on the macroscopic scale, **still remains a significant challenge, especially in numerical simulations.**

Why should we care about the microstructure?

- Traditional numerical methods, such as the finite element method, may **overlook small-scale effects** or **assume homogeneity** that isn't present in real-world materials. Multiscale analysis enables **more accurate predictions by incorporating finer details from smaller scales into the analysis**, leading to more realistic results.
- Considering this microscopic scale provides insights into the **relationship between microscale phenomena and macroscale behavior**. By studying how small-scale features influence overall performance, engineers can optimize designs for specific applications.
- In the case of additive manufacturing, numerical studies may outline **optimal microstructures** targeted for printing.

➤ This is particularly compelling for **aeronautical and space structures**, where an optimal material representation can facilitate **lighter-weight** designs, ultimately **reducing costs**.

Objectives

- Considering the microstructure in a conventional finite element analysis is impractical due to resource constraints.
- While multiscale methods like homogenization attempt to address these challenges, they remain non-industrializable to date.

➤ Hence, a primary 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.

➤ Additionally, another aspect involves constructing an efficient database for the training of such neural networks, based on 3D scans of microstructures.

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

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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**.

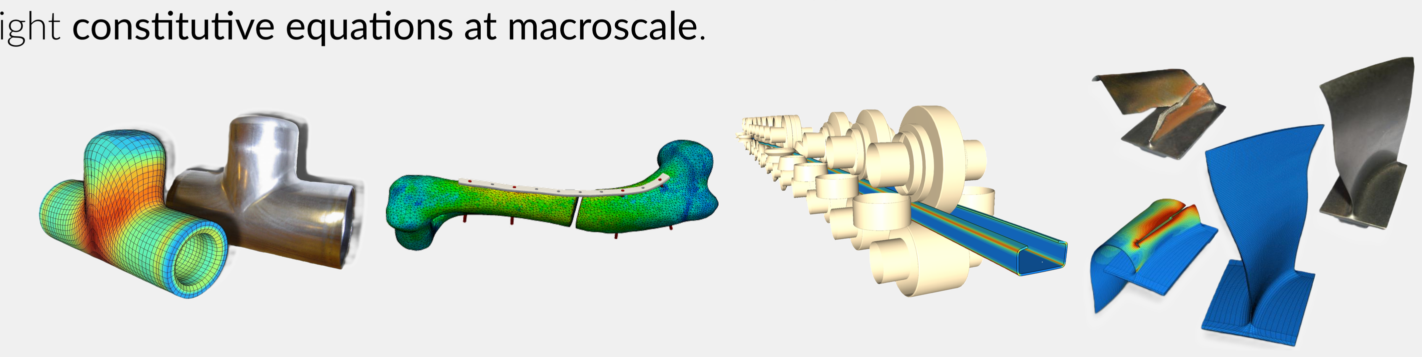

Figure 3. Examples of finite element analysis done with Metafor [3, 2]

Multiscale analysis

- 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**.
- Multiscale methods aim to **mitigate** these demands but still remain, to date, **non-industrializable**.

➤ This thesis is currently based on the finite element squared (FE2) [4]:
  - 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.

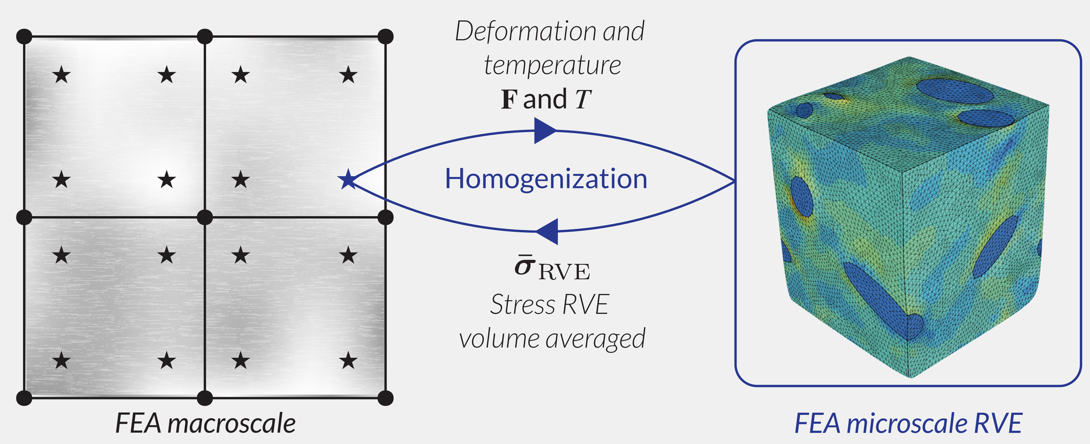

Figure 4. Finite element squared.

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**.

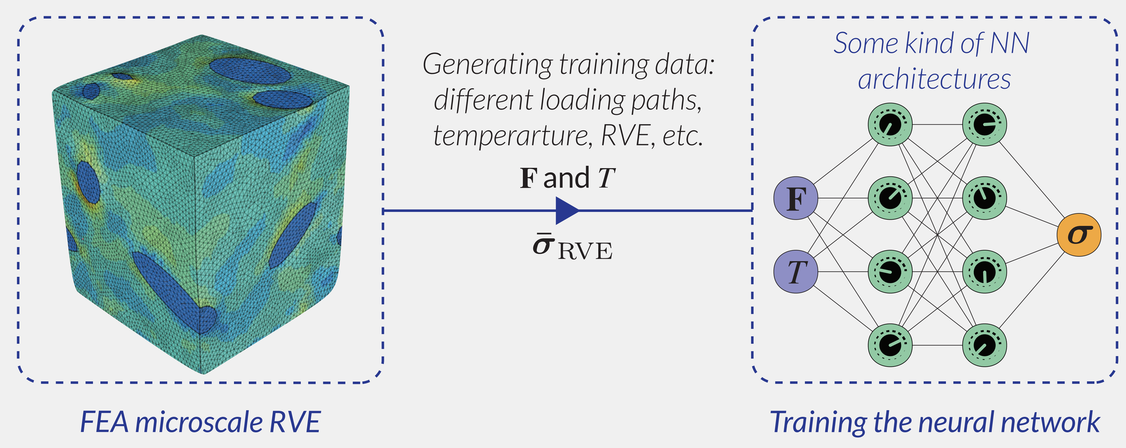

Figure 5. Training a neural network.

➤ 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** compare to vanilla FE2, it is important to consider the **"offline resources"** invested in generating the data and training the neural network.

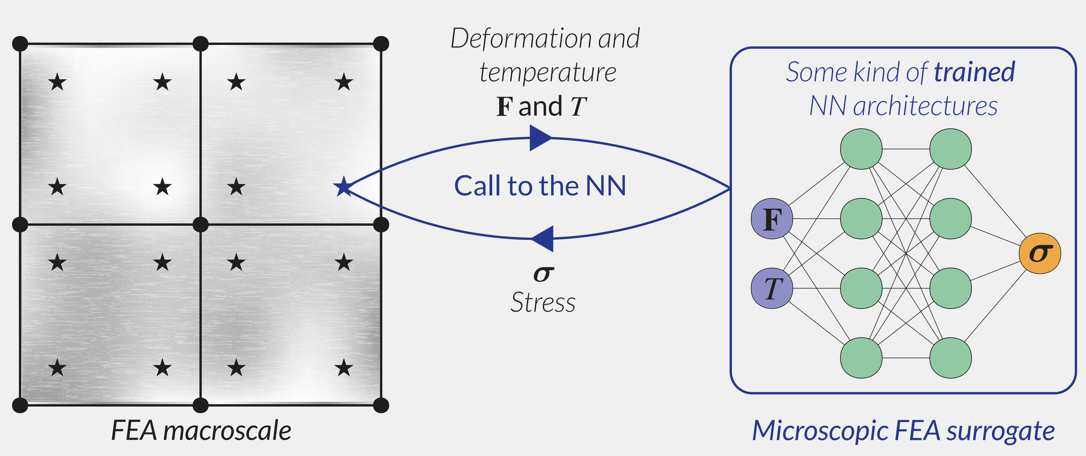

Figure 6. Finite element neural network (FENN).

Current main challenges faced

- Establishing a database for path-dependent materials without resorting to random-walk algorithms for representing deformation paths.
- Neural network architectures capable of handling time sequences with uneven spacing.
- The inner workings of advanced neural networks often remain opaque, resembling a black box, where understanding how inputs translate into outputs can be challenging.
- Convergence of the Newton-Raphson procedure with the finite element squared.
- Extending current mechanical results to thermomechanical simulations.

Space4Relaunch

Ph.D. Day, UCLouvain — February 7, 2024

The present research is part of the Space4ReLaunch project, which is supported by the SPW Economie Emploi Recherche of the Walloon Region, under the grant agreement n°2210181.