Efficient multiscale simulations of additively manufactured alloys at finite strain: Towards a hybrid approach combining FE-NN and FE^2

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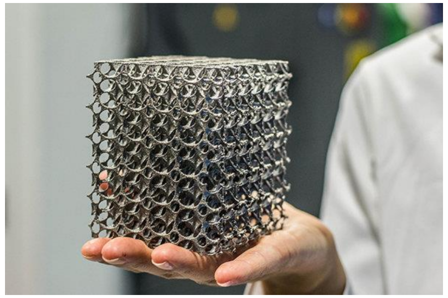
Outline

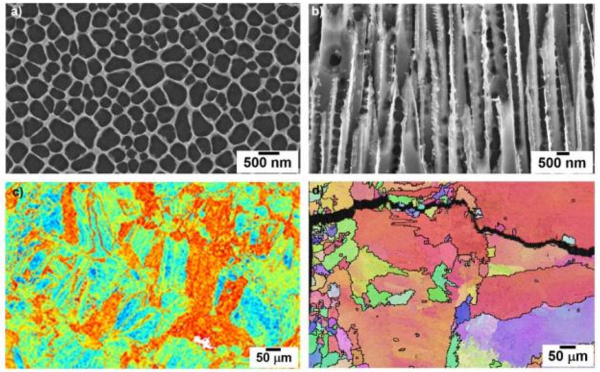
- Background & Motivation
- Finite element squared in our in-house FE code Metafor
  - → *Challenge 1: Efficiency & robustness*
- A hybrid approach combining FE-NN and FE^2
  - → *Challenge 2: Reducing cost while preserving reliability of multiscale simulations*
- Conclusion and future perspectives

Background & Motivation



- Context
  - Additive Manufacturing (AM) holds promising prospects in the space sector, particularly within the "New Space" movement, which emphasizes the use of miniature satellites (CubeSats), reusable launchers, and more.

- Advantages of AM
  - AM enables the design of innovative structures, unlocking new design possibilities:
    - Optimized and constructed in a single piece.
    - Unachievable with conventional methods.



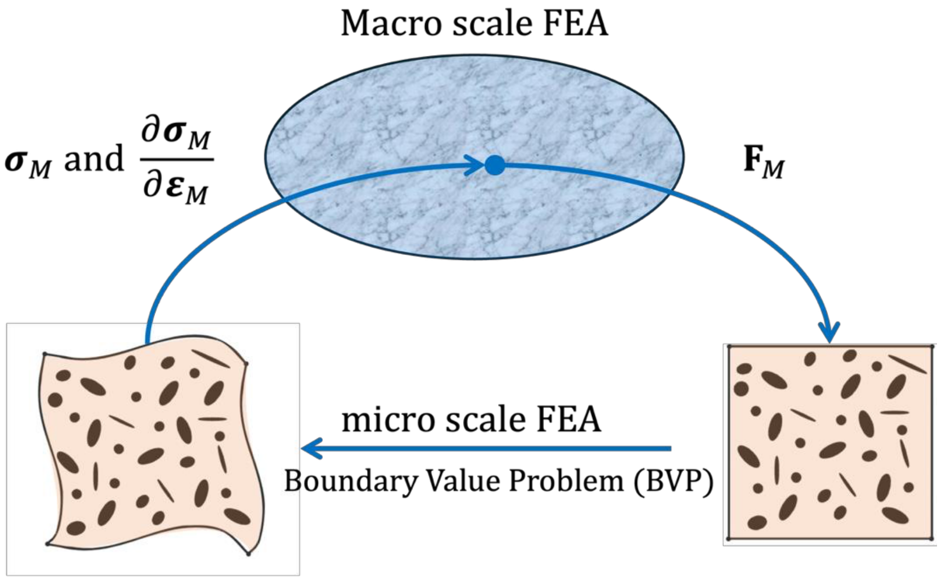
- Challenges
  - However, AM introduces new challenges due to the microstructure it generates, including gaps, porosities, inclusions, etc., which can influence the material's strength.

Reality is complex!

Multiscale simulations: Finite Element Squared (FE²)

The key idea is to include smaller scale effects while avoiding "large" FE simulations.

- There are two scales simultaneously:
  - Macroscopic scale (M): Mechanical part
  - microscopic scale (m): 3D scans, RVE, etc.



- Hill–Mandel macro-homogeneity condition:

Virtual work *of a Macro point* → A Macro Gauss point	$\mathbf{P}_M : \delta \mathbf{F}_M = \frac{1}{V_0} \int_{V_0} \mathbf{P}_m : \delta \mathbf{F}_m \, dV_0$	Virtual work averaged *of a micro volume* → its micro FEA (BVP)

→ Specific boundary conditions @micro

- Scale transition:
  - $\mathbf{F}_M = \frac{1}{V_0} \int \mathbf{F}_m dV_0 \rightarrow \mathbf{F}_m = \mathbf{F}_M + \tilde{\mathbf{F}}$
  - $\mathbf{P}_M = \frac{1}{V_0} \int \mathbf{P}_m dV_0$ (or $\boldsymbol{\sigma}_M = \frac{1}{V} \int \boldsymbol{\sigma}_m dV$)

Challenge 1: An efficient FE² code

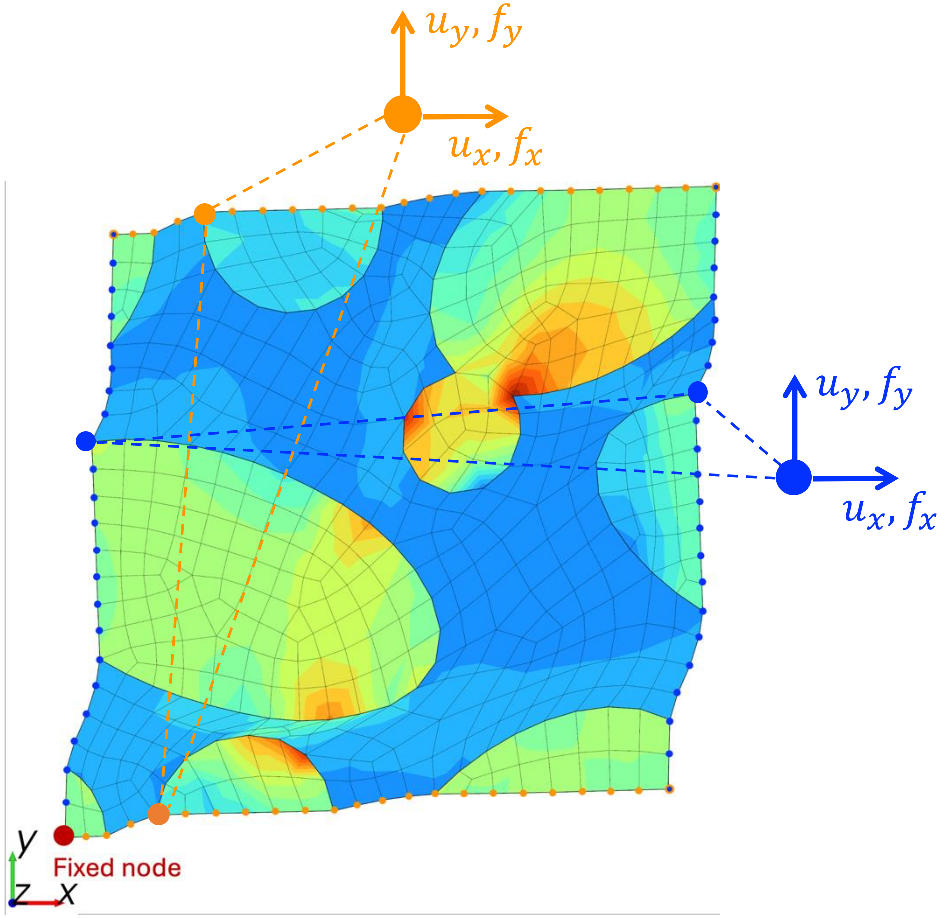
Multiscale simulations such as FE² are **inherently computationally expensive.**

- To mitigate this intrinsic cost:
  - Multiple microscale boundary value problems in parallel.
  - Consistent macroscopic tangent moduli operator $\frac{\partial \boldsymbol{\sigma}_M}{\partial \boldsymbol{\varepsilon}_M}$ → better convergence.
  - Reduced computational cost associated with $\boldsymbol{\sigma}_M$ and $\frac{\partial \boldsymbol{\sigma}_M}{\partial \boldsymbol{\varepsilon}_M}$ thanks to the master nodes.
- All developments have been integrated into Metafor, our in-house nonlinear finite element solver:
  - finite strain
  - updated Lagrangian,
  - hypoelastic formulation,
  - Jaumann rate of the Cauchy stress.

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/.

Challenge 1: An efficient FE² code, the master nodes

Periodic boundary conditions are imposed between opposite faces using Lagrange multipliers, driven by the displacements of their associated master node.



- From $\mathbf{F}_\mathrm{M}$, displacements $\boldsymbol{u}$ are imposed on the two (2D) or three (3D) master nodes, driving the microscale boundary value problem:

$$\begin{cases} u_y^1 - u_y^0 = u_y \\ u_y^1 - u_y^0 = u_y \end{cases} \qquad \begin{cases} u_y^1 - u_y^0 = u_y \\ u_y^1 - u_y^0 = u_y \end{cases}$$

The full macroscopic response is obtained from the two (2D) or three (3D) master nodes.

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

$$\mathbf{K}_{\mathrm{S.E.}} = \frac{\partial f}{\partial \boldsymbol{u}} \Rightarrow [\dots] \Rightarrow \frac{\partial \boldsymbol{\sigma}_M}{\partial \boldsymbol{\varepsilon}_M}$$

Challenge 1: An efficient FE² code, the master nodes

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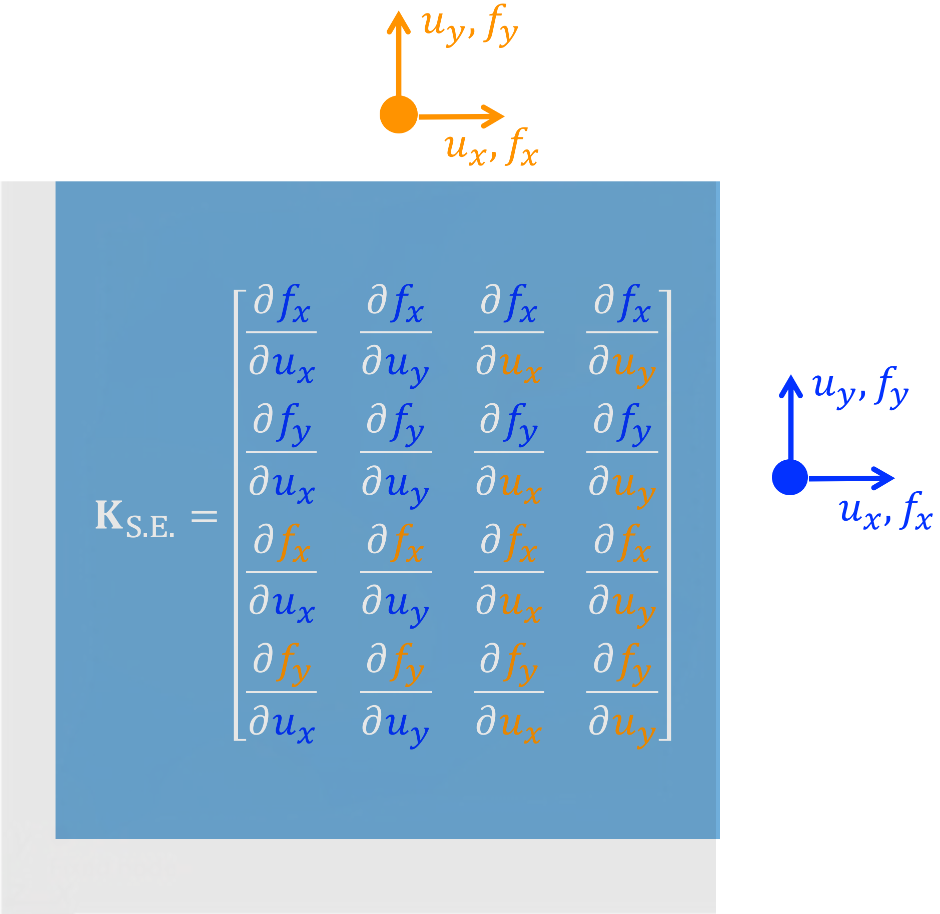

$$\mathbf{K}_{\text{S.E.}} = \begin{bmatrix} \frac{\partial f_x}{\partial u_x} & \frac{\partial f_x}{\partial u_y} & \frac{\partial f_x}{\partial u_x} & \frac{\partial f_x}{\partial u_y} \\ \frac{\partial f_y}{\partial u_x} & \frac{\partial f_y}{\partial u_y} & \frac{\partial f_y}{\partial u_x} & \frac{\partial f_y}{\partial u_y} \\ \frac{\partial f_x}{\partial u_x} & \frac{\partial f_x}{\partial u_y} & \frac{\partial f_x}{\partial u_x} & \frac{\partial f_x}{\partial u_y} \\ \frac{\partial f_y}{\partial u_x} & \frac{\partial f_y}{\partial u_y} & \frac{\partial f_y}{\partial u_x} & \frac{\partial f_y}{\partial u_y} \end{bmatrix}$$

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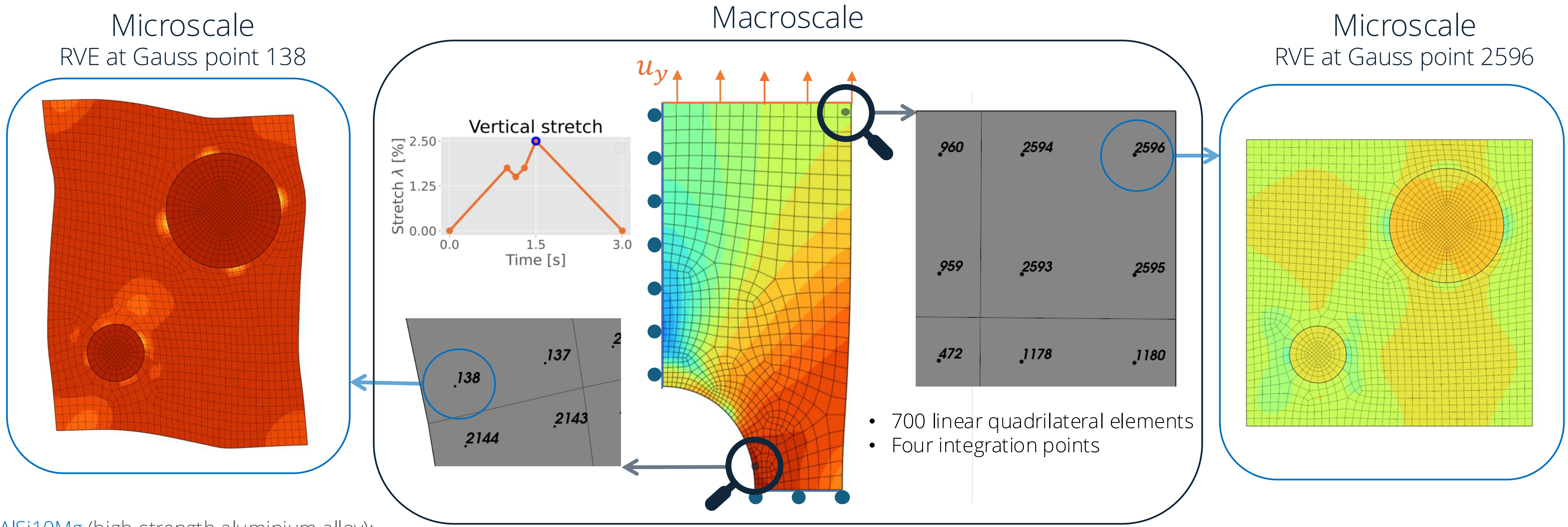
Metafor: an efficient plane strain and 3D FE^2 solver



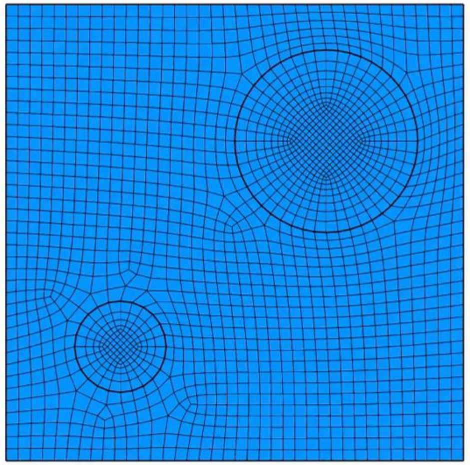
AlSi10Mg (high-strength aluminium alloy):
- Matrix: Elastoplastic + nonlinear hardening
- Particles: Elastic
- 2,200 linear quadrilateral elements

Metafor: an efficient plane strain and 3D FE² solver

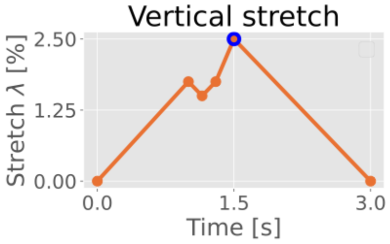
120 steps were computed, requiring 165 (macro) iterations and **1h50 using 64 cores**.

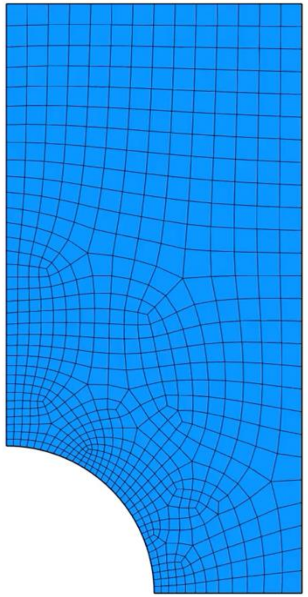
Microscale

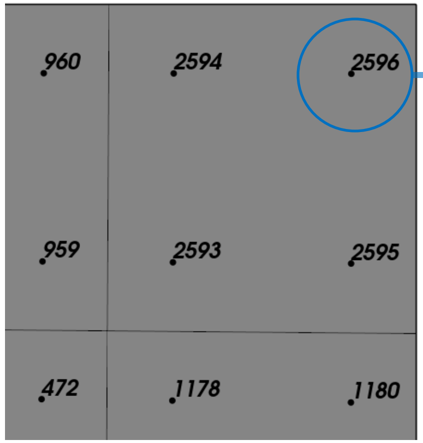
RVE at Gauss point 138



Macroscale



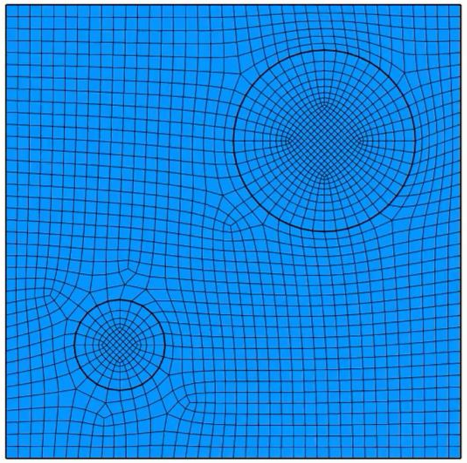




- 700 linear quadrilateral elements
- Four integration points

Microscale

RVE at Gauss point 2596



AlSi10Mg (high-strength aluminium alloy):
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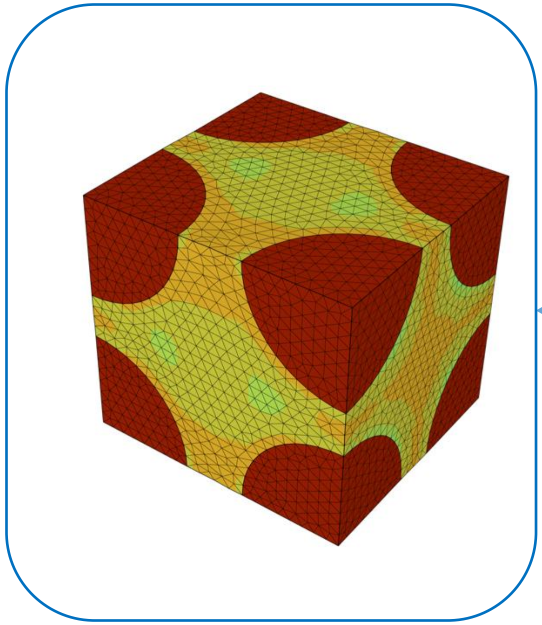
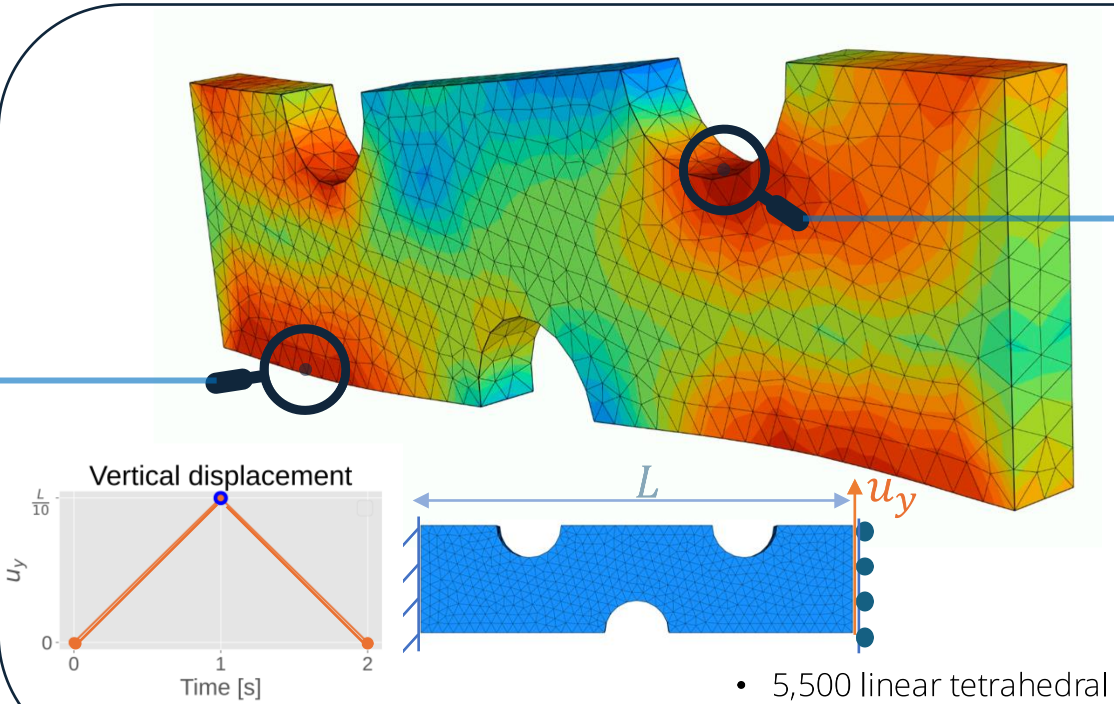
Equivalent von Mises stress

Metafor: an efficient plane strain and 3D FE^2 solver

Microscale
RVE at Gauss point 138

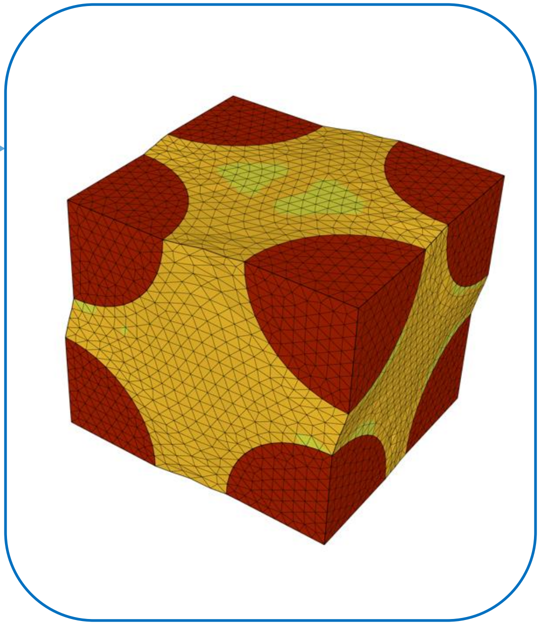


Macroscale



- 5,500 linear tetrahedral elements
- Single integration point

Microscale
RVE at Gauss point 2596



AlSi10Mg (high-strength aluminium alloy):

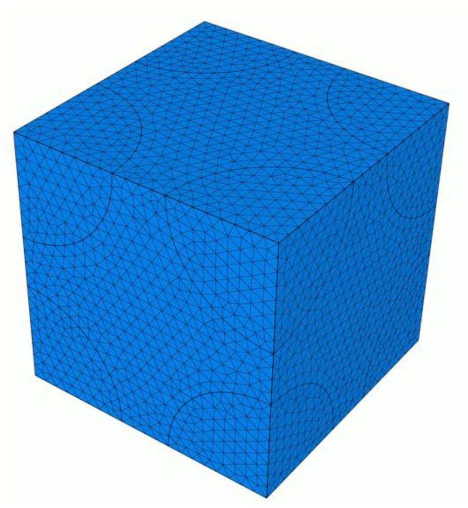
- Matrix: Elastoplastic + nonlinear hardening
- Particles: Elastic
- 43,000 linear tetrahedral elements

Metafor: an efficient plane strain and 3D FE^2 solver

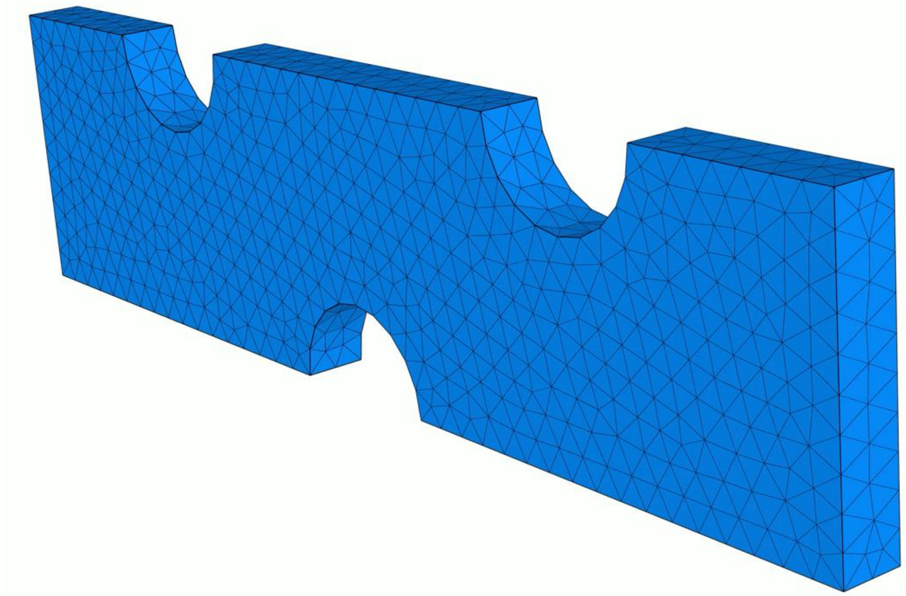
75 steps were computed, requiring 127 (macro) iterations and **47h20 using 64 cores**.

Microscale

RVE at Gauss point 138



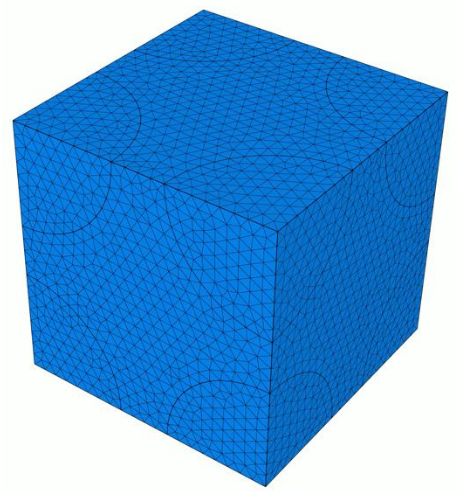
Macroscale



- 5,500 linear tetrahedral elements
- Single integration point

Microscale

RVE at Gauss point 2596



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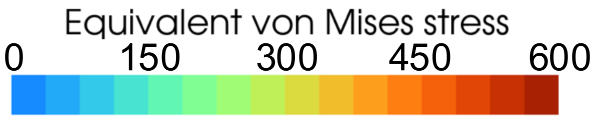


Challenge 2: combine FE² with deep learning

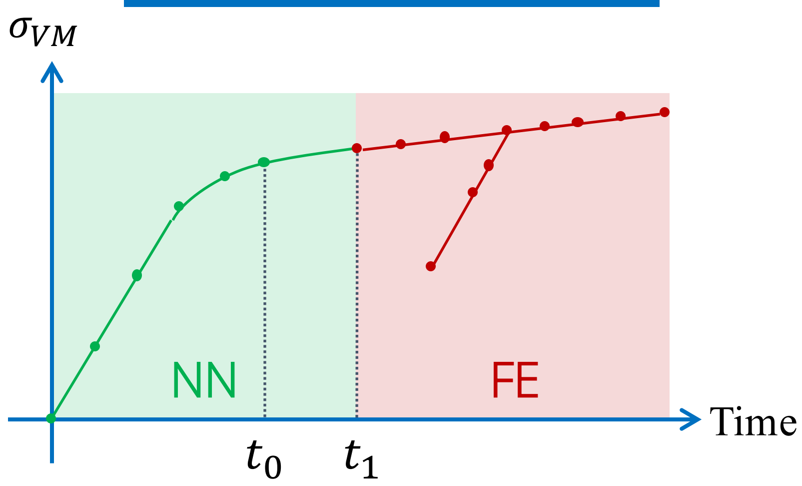
Multiscale simulations such as FE² are **inherently computationally expensive.**

- Neural Networks (NN) – *once properly trained* – can be employed to reduce the computational cost of the microscale simulations → FE-NN.
  - Offline cost associated with training the model and generating the data.
  - NN will never be able to extrapolate *infinitively* beyond their training data.
  - A complex neural network architectures may not be an effective strategy,
  - nor relying solely on neural networks for multiscale simulations.

A promising direction could lie in **a hybrid approach, combining the efficiency of neural networks FE-NN with the reliability of traditional FE².**

The FE-NN–FE² Hybrid Approach: concept and applicability

For a given **Macro** GP



(Converged) Step at t_0

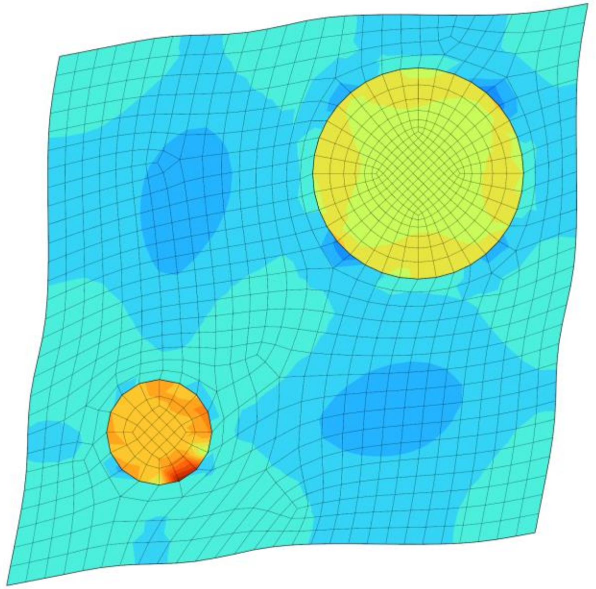
Step at t_1	
Iteration	Convergence
0 (FE)	no
1 (NN)	no
2 (FE)	**YES!**

- At time t=0, all macro Gauss points (GP) use the neural network surrogate model to predict microscale responses.
- During the simulation, **some macro Gauss points may switch** to the FEA of the RVE if the local loading conditions fall outside the neural network's training data.

- The NN surrogate must be:
  - Be trained on a well-defined dataset (no random walk algorithms) → switching criterion.
  - As simple as possible (avoiding black-box architectures).

The FE-NN–FE² Hybrid Approach: elastic domain of an elastoplastic RVE

AlSi10Mg *(high-strength aluminium alloy)*:
- Matrix: Elastoplastic + nonlinear hardening
- Particles: Elastic



As for the homogenized stress:

$$\bar{\varepsilon}^p_M = \frac{1}{v}\int_v \bar{\varepsilon}^p_m \, dv \implies \eta = \begin{cases} 1 & \bar{\varepsilon}^p_M > 0 \\ 0 & \text{otherwise} \end{cases}$$

- The switching criterion is triggered when plasticity occurs in the RVE.
- → Before path dependency: a simple feed-forward neural network $\mathcal{N}$ can be used.
- $\mathcal{N}$ has been trained to identify whether $\boldsymbol{\varepsilon}_M$ falls within the plastic region.

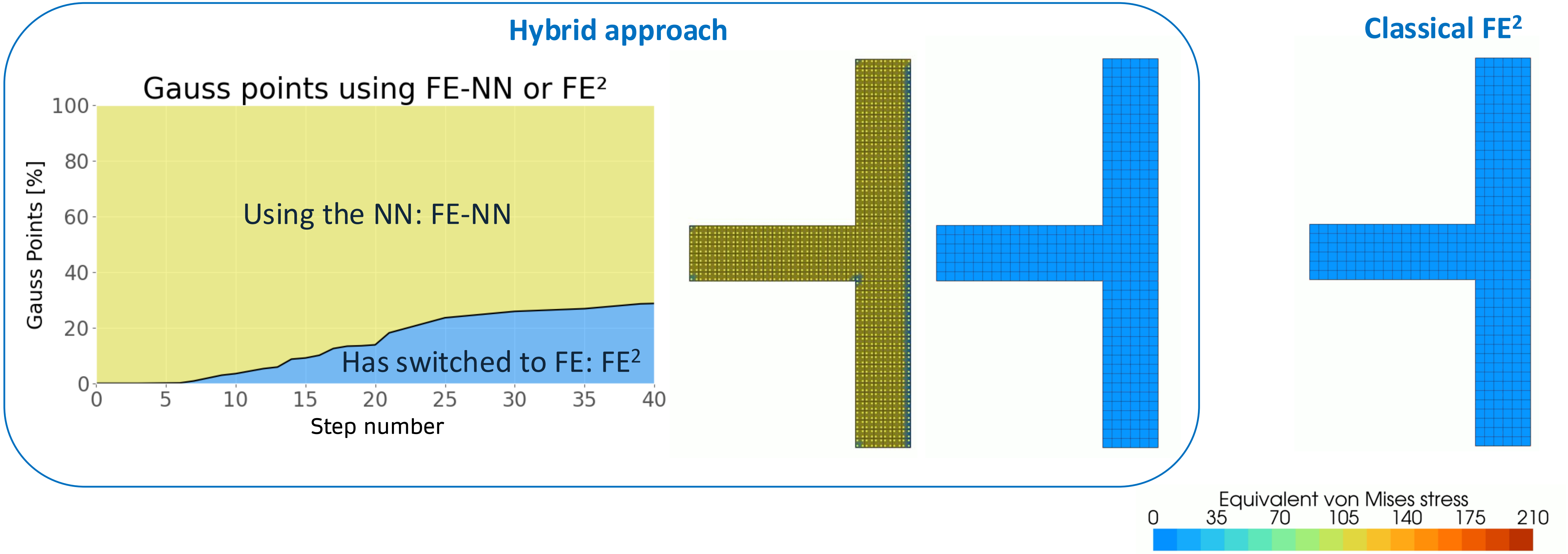
$$\boldsymbol{\sigma}_M, \eta = \mathcal{N}(\boldsymbol{\varepsilon}_M)$$

$\boldsymbol{\eta} = \mathbf{0}$ → Elastic region: can rely on $\mathcal{N}$'s prediction.

$\boldsymbol{\eta} > \mathbf{0}$ → Plasticity occurred: switching from $\mathcal{N}$ to FE.

The FE-NN–FE² Hybrid Approach: result (1)

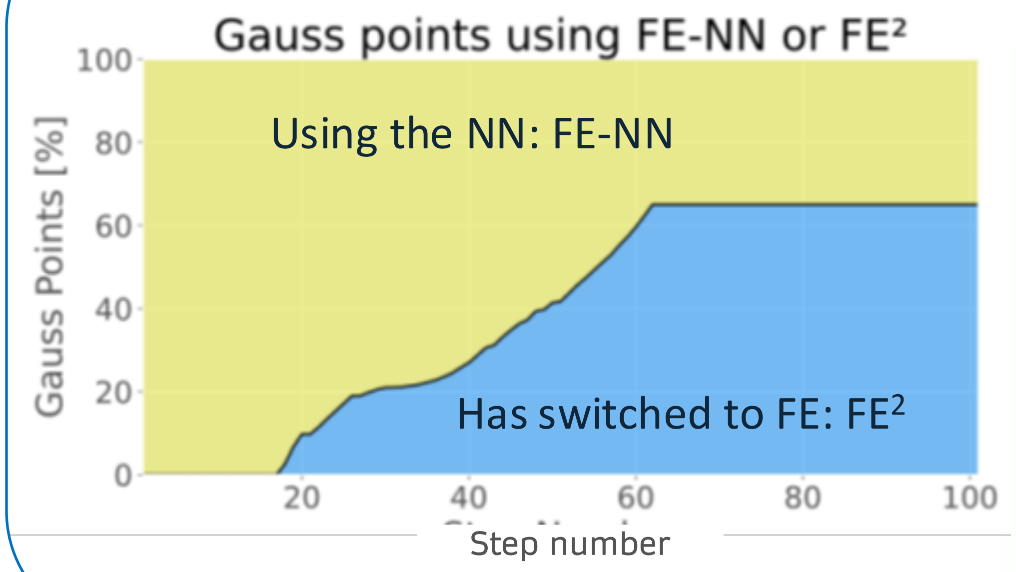
- **Offline:** 40 min to generate the data and training the model *(5 cores)*
- **Online: 3 min for** FE-NN–FE² compared **to 40 min** for FE² *(10 cores)* → 12.3× speed-up *(and 80x less disk space!)*

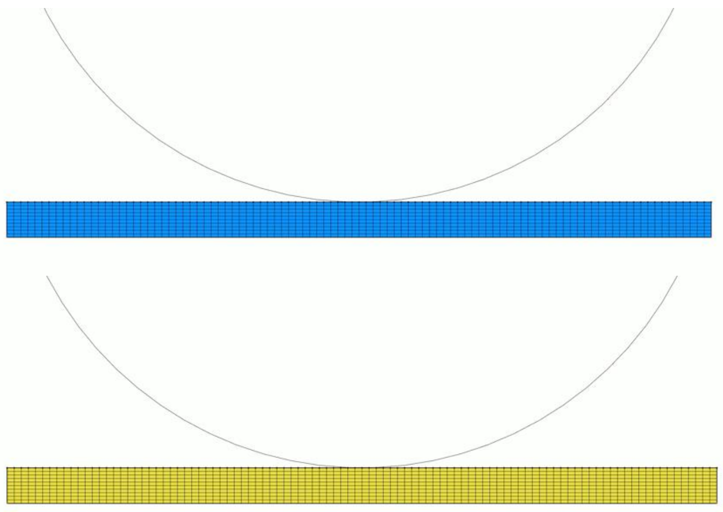


The FE-NN–FE^2 Hybrid Approach: result (2)

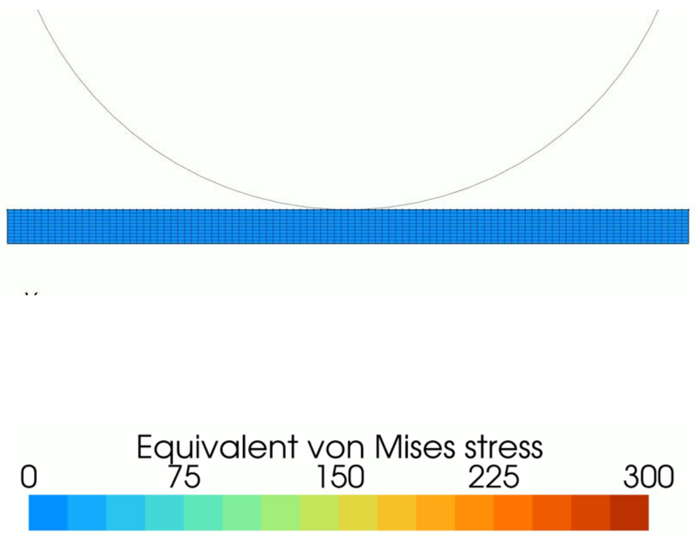
- **Offline:** 40 min to generate the data and training the model *(5 cores)*
- **Online: 140 min for** FE-NN–FE^2 compared **to 180 min** for FE^2 *(10 cores)* → 1.3× speed-up *(and 20x less disk space!)*

Hybrid approach





Classical FE^2

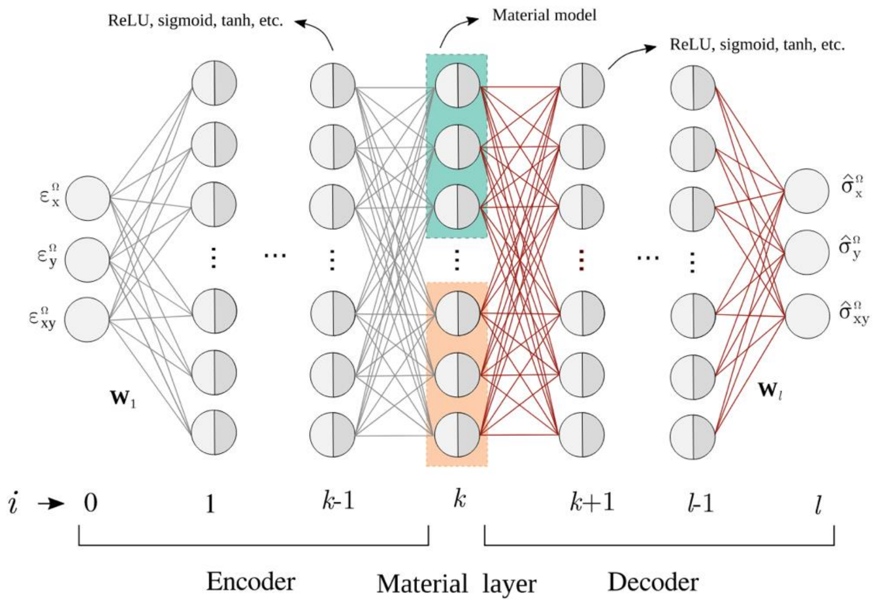


Challenge 2: extension to path-dependent region

- Classical Recurrent Neural Networks (LSTM, GRU, MGRU, etc.) ?
  - Self-inconsistent, strain increment size dependence, lots of internal parameters → expensive training.
  - History variables: little to no physical meaning.
  - Trained on random-walk-generated paths → how to define the switching criterion?

- Physically Recurrent Neural Networks (PRNN) *(M.A. Maia et al., 2023)*
  - Self-consistent, strain increment size independence, very few internal parameters → inexpensive training.
  - History variables: fictitious material models in the NN.
  - Predict unloading/reloading behavior when trained **monotonic data.**

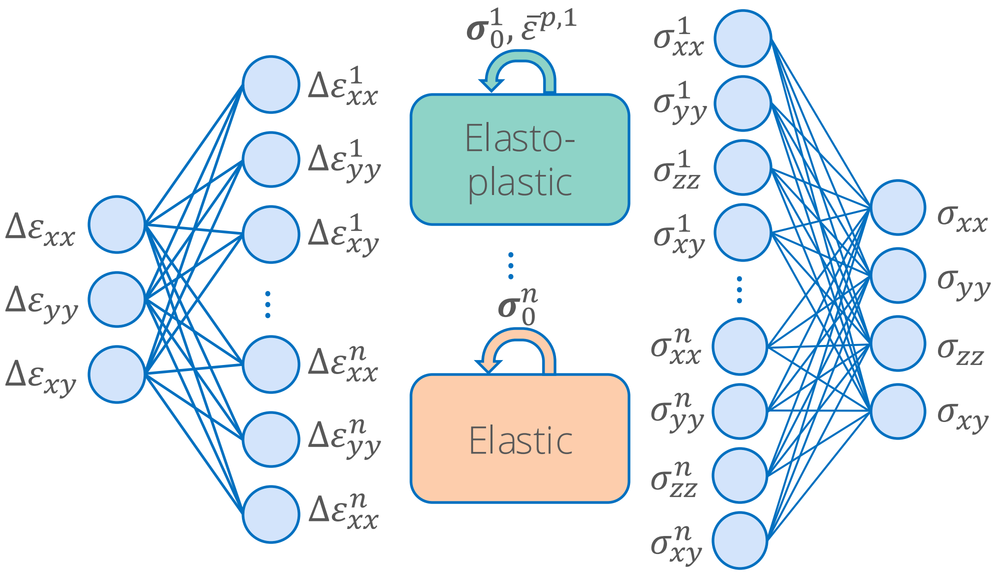
  No random-walk-generated paths → switching criterion ✓



M.A. Maia, I.B.C.M. Rocha, D. Kovačević, and F.P. Van Der Meer. 'Physically Recurrent Neural Network for Rate and Path-Dependent Heterogeneous Materials in a Finite Strain Framework'. Mechanics of Materials 198 (2024)
M.A. Maia, I.B.C.M. Rocha, P. Kerfriden, and F.P. Van Der Meer. 'Physically Recurrent Neural Networks for Path-Dependent Heterogeneous Materials: Embedding Constitutive Models in a Data-Driven Surrogate'. CMAME 407 (2023)

Challenge 2: extension to path-dependent region

- The PRNN used in this hybrid approach is highly inspired by *M.A. Maia et al. (2024)* , with the following adaptations:
  - Input: logarithm strain increment $\Delta\boldsymbol{\varepsilon}_M$.
  - Encoder and decoder are a linear layer without bias: $\Delta\boldsymbol{\varepsilon} = \mathbf{0} \rightarrow \Delta\boldsymbol{\sigma} = \mathbf{0}$.
  - The same material models and radial return algorithm as those implemented in Metafor.
- Each macro GP stores its loading history + the history variables of the n material models.



The FE-NN–FE² Hybrid Approach: extension to path-dependent region

Application: A macroscopic simulation under monotonic loading, with a RVE (¼ elastic and ¾ elastoplastic with saturated hardening materials).

- Knowing this application, the PRNN is:
  - Composed of the same material ratio.
  - Trained on monotonic loadings (100 paths with $\|\boldsymbol{\varepsilon}\| = 10\%$); following *M.A. Maia et al. (2024).*
  - Offline phase 60 min: 20 min to generate the data, 40 min to train the model on a single core.
  - Tested within this range, the PRNN predicts loading/unloading as in *M.A. Maia et al. (2024)*

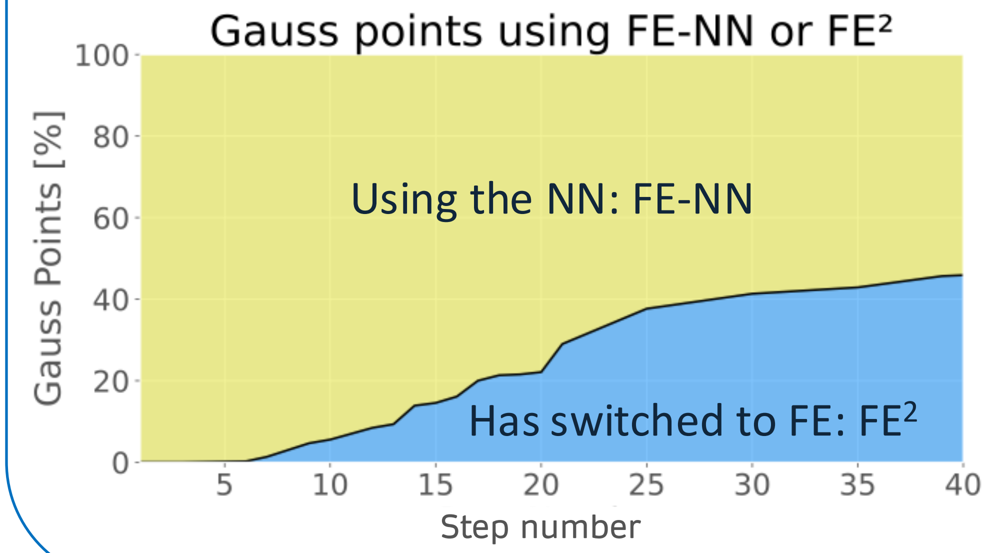
→ Monotonic loading @Macro but GP may see loading/unloading.

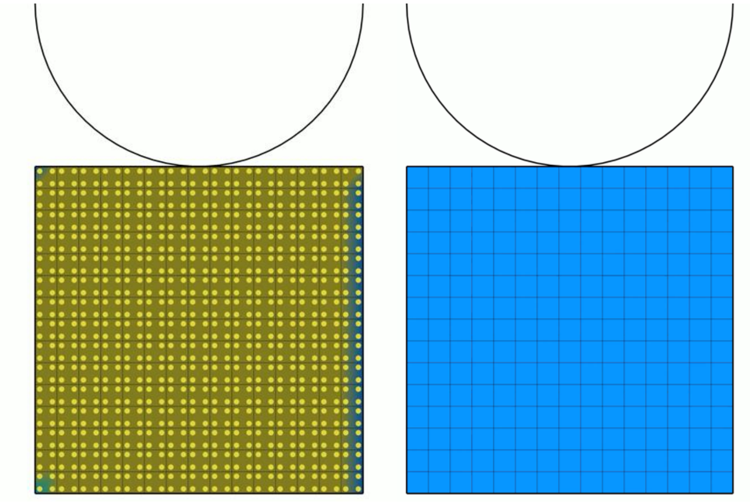
- The hybrid approach for this application:
  - Switching criterion: when the macro strain norm exceeds $\|\boldsymbol{\varepsilon}_M\| > 9\%$.
  - $\frac{\partial \boldsymbol{\sigma}_M}{\partial \boldsymbol{\epsilon}_M}$ from backpropagation (more efficient than finite difference).

The FE-NN–FE² Hybrid Approach: extension to path-dependent region

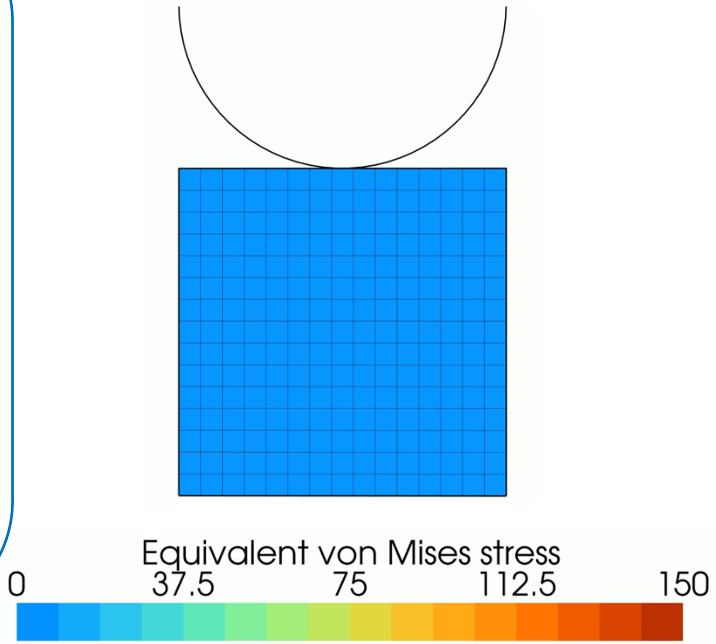
- **Offline:** 60 min to generate the data (100 monotonic paths) and training the PRNN on a single core.
- **Online:** 120 min for FE-NN–FE² compared to 170 min for FE² *(10 cores)* → 1.4× speed-up *(and 10x less disk space!)*

Hybrid approach





Classical FE²



Conclusion and future perspectives

- Multiscale simulations such as FE² are inherently expensive:
  - Importance of an efficient implementation and robust approximation of $\frac{\partial \sigma_M}{\partial \varepsilon_M}$.
- We proposed a hybrid approach:
  - Combines the efficiency of neural networks in specific ranges,
  - while switching to a FEA of the microscale once we can no longer rely on the NN.

  → Reduces online cost compared to vanilla FE².

  → Reduces offline cost compared to vanilla FE-NN.

  → The user has the control of the neural network.
- Future directions:
  - Extend this hybrid approach to broader loading path coverage.
  - Apply both methods (FE² + hybrid) to real mechanical tests on AM parts.

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Wallonie

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