Groupe de recherche 3MAH

Opérateurs en champs moyens et apports de l'IA pour l'homogénéisation non-linéaire

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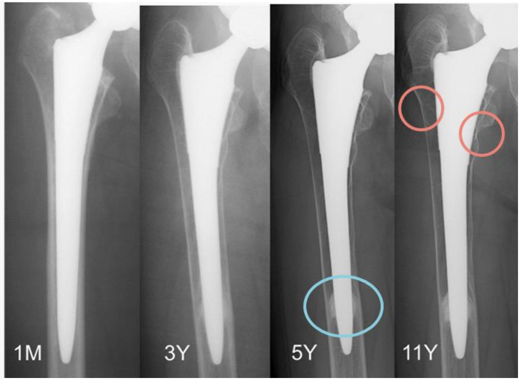
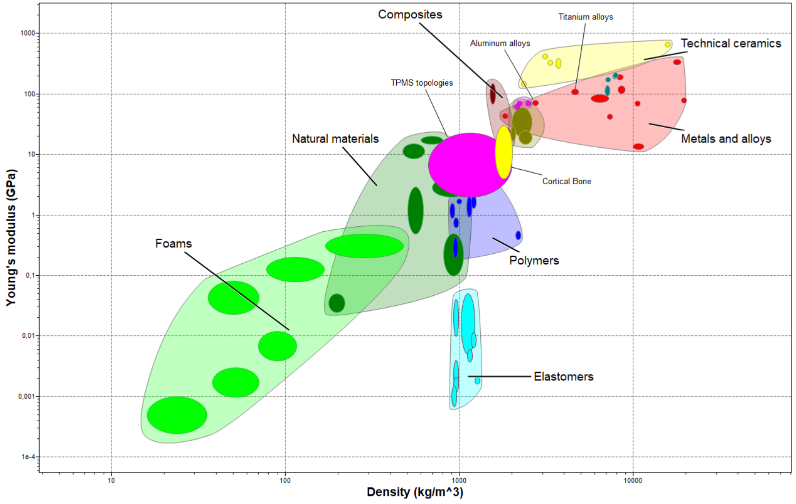
Context : A need for better mechanical compatibility

[1]



The effect of stress shielding on the peri-implant bone [2]

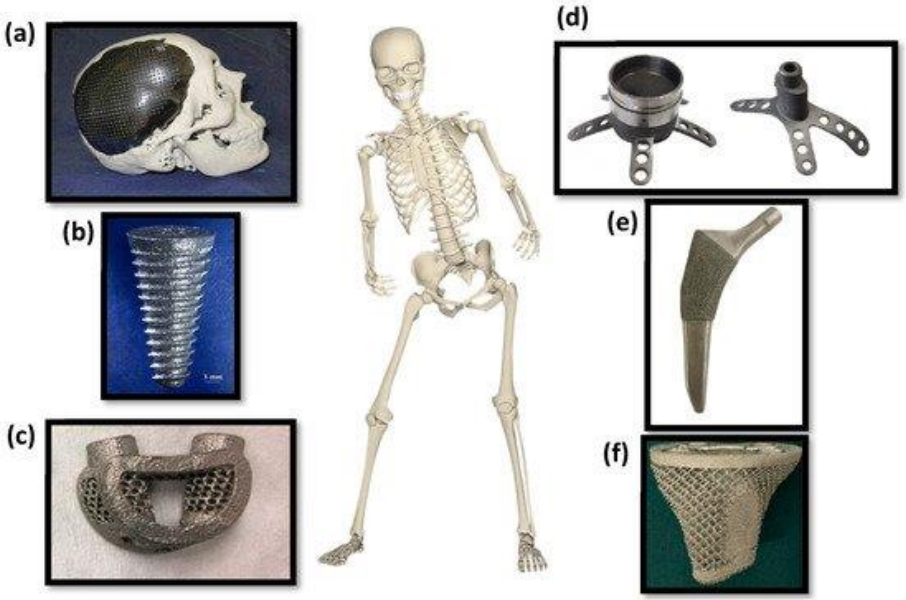


Hard to find replacement materials! [3]

Young modulus of implant >> Young modulus of Cortical bone

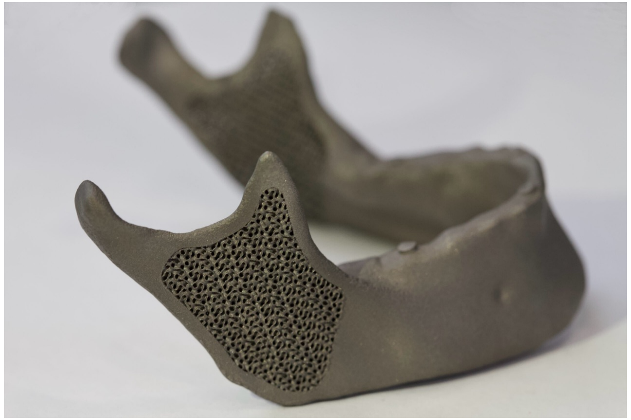
[1]'https://www.coastlineortho.com/joint-replacement-surgery-coastline-orthopaedic-associates.html'
[2] M. Fischer, PhD Thesis, Universite de Lorraine, 2017
[3] C. Chatzigeorgiou, PhD Thesis, ENSAM, 2017

Context : A need for better mechanical compatibility



I. Buj-Corral et al. 2020

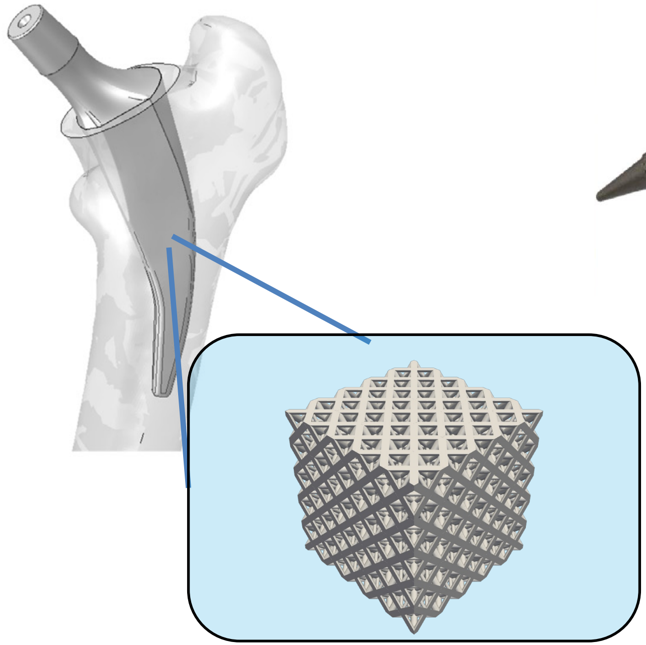
Y. He, et al. 2018



Pint.fr

Use of architectured material can improve biocompatibility

The difficulty to simulate : A multiscale approach



Direct Finite Element simulation:
Computationally very expensive!

Repetitive number of cells:

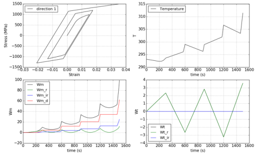
↓

Periodic arrangement

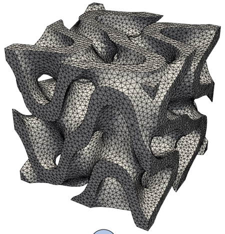
↓

Periodic homogenization

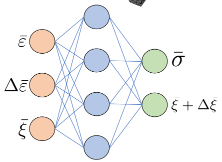
Ingredients



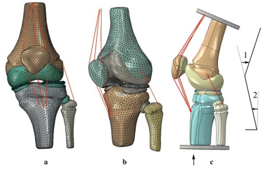
Constitutive models



Homogenization



IA-physics models



Advanced simulation

3MAH Team

https://github.com/3MAH

Non-linear homogenization : local law

Clausius-Duhem inequality: $\gamma = \boldsymbol{\sigma} : \dot{\varepsilon} + \theta\dot{\eta} - \dot{E} - \frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{\nabla\theta} \geq 0,$ ➡ $\gamma = \gamma_{\text{loc}} + \gamma_{\text{con}} \geq 0,$

$$\gamma_{\text{loc}} = \boldsymbol{\sigma} : \dot{\varepsilon} + \theta\dot{\eta} - \dot{E}, \quad \gamma_{\text{con}} = -\frac{\boldsymbol{q}}{\theta} \cdot \boldsymbol{\nabla\theta}.$$

Legendre-Fenchel transformation + Germain (1983) : Convexity of E

$G(\boldsymbol{\sigma}, \theta, \zeta) := E - \theta\eta - \boldsymbol{\sigma} : \boldsymbol{\varepsilon}$ $\quad \boldsymbol{\varepsilon} = -\frac{\partial G}{\partial \boldsymbol{\sigma}} \quad \eta = -\frac{\partial G}{\partial \theta}$ ➡ $\gamma_{\text{loc}} = -\frac{\partial G}{\partial \zeta} : \dot{\zeta}$

M mechanisms are considered , with a set of N_m variables for each mechanism: $\{\boldsymbol{V}_i^m\}$

Generalized thermodynamic forces $\boldsymbol{A}_{\boldsymbol{V}_i^m} = -\frac{\partial G}{\partial \boldsymbol{V}_i^m}$

A criterion is associated with each mechanism : Example $\Phi^m\left(\{\boldsymbol{A}_{\boldsymbol{V}}{}^m\}\right) \leq 0$

$$\{\Phi^m\} \leq \{0\}, \quad \{\dot{s}^m\} \geq \{0\}, \quad \{\Phi^m \dot{s}^m\} = 0$$

Non-linear homogenization : local law

Increment in time of a quantity

$$x^{(n+1)} = x^{(n)} + \Delta x^{(n+1)}$$

Increment of a quantity for an iteration m

$$\Delta x^{(n+1)(m+1)} = \Delta x^{(n+1)(m)} + \eth x^{(n+1)(m)}$$

Increment of a quantity for an iteration k inside the iteration m

$$\Delta x^{(n+1)(m+1)(k+1)} = \Delta x^{(n+1)(m+1)(k)} + \delta x^{(n+1)(m+1)(k)}$$

Local constitutive law

$$\begin{aligned} \boldsymbol{\varepsilon}^{(n+1)(m+1)} &= \boldsymbol{\varepsilon}^{(n)} + \Delta\boldsymbol{\varepsilon}^{(n+1)(m+1)}, \\ \theta^{(n+1)(m+1)} &= \theta^{(n)} + \Delta\theta^{(n+1)(m+1)}, \\ \zeta^{(n+1)(m+1)} &= \zeta^{(n)}. \end{aligned}$$

$$\delta\boldsymbol{\varepsilon}^{(n+1)(m+1)(k)} = 0, \quad \delta\theta^{(n+1)(m+1)(k)} = 0$$

$$\begin{aligned} \eth\boldsymbol{\sigma} &= \boldsymbol{\mathcal{L}} : \left(\eth\boldsymbol{\varepsilon} - \eth\boldsymbol{\varepsilon}^{\text{th}} - \eth\boldsymbol{\varepsilon}^{\text{in}}\right) \\ \eth r &= -\eth\theta\frac{\Delta\eta}{\Delta t} - \theta\frac{\eth\eta}{\Delta t} + \eth\gamma_{\text{loc}} \\ \eth\gamma_{\text{loc}} &= \eth\boldsymbol{A}_\zeta\frac{\Delta\zeta}{\Delta t} + \boldsymbol{A}_\zeta\frac{\eth\zeta}{\Delta t} \end{aligned}$$

Non-linear homogenization : local law

Increment in time of a quantity

$$x^{(n+1)} = x^{(n)} + \Delta x^{(n+1)}$$

Increment of a quantity for an iteration m

$$\Delta x^{(n+1)(m+1)} = \Delta x^{(n+1)(m)} + \eth x^{(n+1)(m)}$$

Increment of a quantity for an iteration k inside the iteration m

$$\Delta x^{(n+1)(m+1)(k+1)} = \Delta x^{(n+1)(m+1)(k)} + \delta x^{(n+1)(m+1)(k)}$$

Local constitutive law

$$\begin{aligned} \boldsymbol{\varepsilon}^{(n+1)(m+1)} &= \boldsymbol{\varepsilon}^{(n)} + \Delta\boldsymbol{\varepsilon}^{(n+1)(m+1)}, \\ \theta^{(n+1)(m+1)} &= \theta^{(n)} + \Delta\theta^{(n+1)(m+1)}, \\ \zeta^{(n+1)(m+1)} &= \zeta^{(n)}. \end{aligned}$$

$$\delta\boldsymbol{\varepsilon}^{(n+1)(m+1)(k)} = 0, \quad \delta\theta^{(n+1)(m+1)(k)} = 0$$

$$\boldsymbol{D}^{\varepsilon} = \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}} \qquad \boldsymbol{D}^{\theta} = \frac{\partial\boldsymbol{\sigma}}{\partial\theta}$$

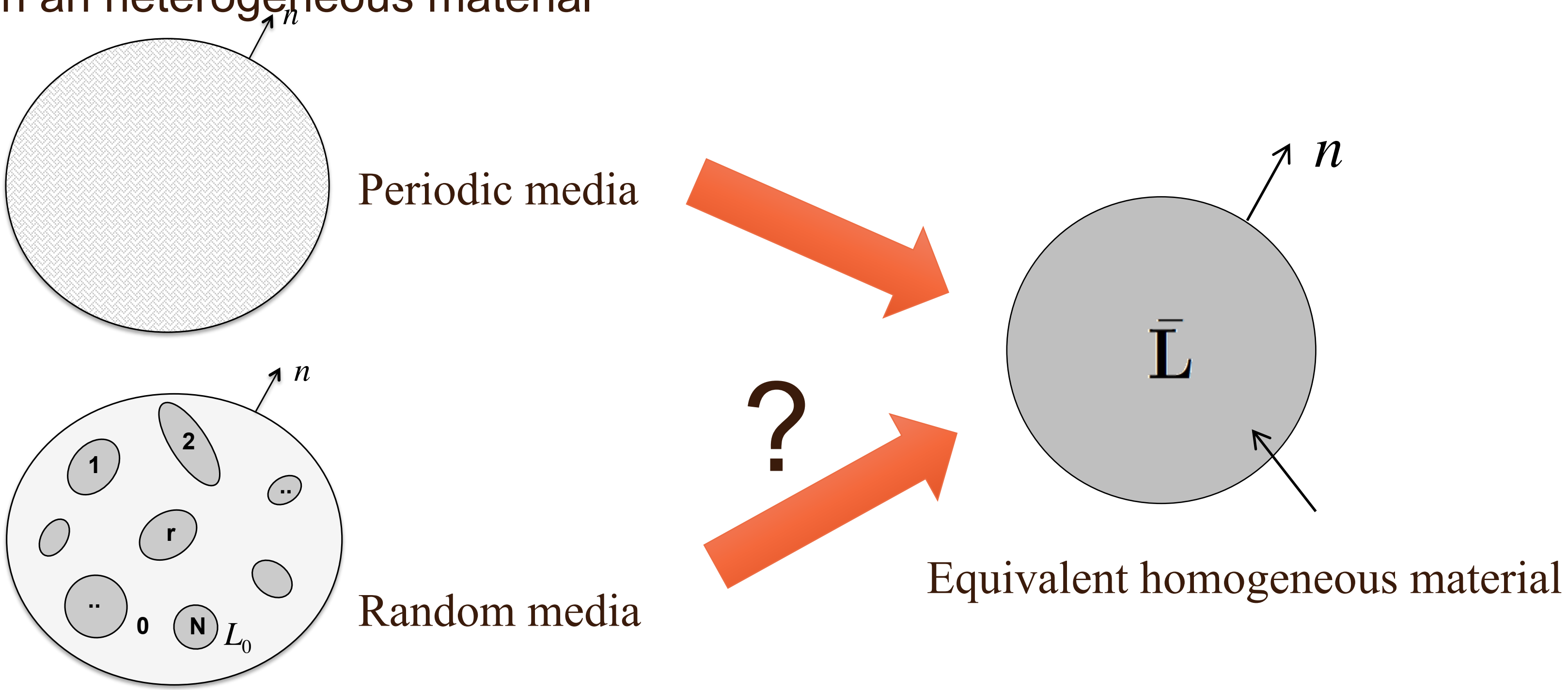
$$\boldsymbol{R}^{\varepsilon} = -\frac{\partial Q}{\partial\boldsymbol{\varepsilon}} = \frac{\partial r}{\partial\boldsymbol{\varepsilon}} \qquad R^{\theta} = -\frac{\partial Q}{\partial\boldsymbol{\theta}} = \frac{\partial r}{\partial\boldsymbol{\theta}}$$

$$\eth\boldsymbol{\sigma} = \boldsymbol{D}^{\varepsilon}:\eth\boldsymbol{\varepsilon} + \boldsymbol{D}^{\theta}\eth\bar{\theta} \qquad \eth r = \boldsymbol{R}^{\varepsilon}:\eth\boldsymbol{\varepsilon} + R^{\theta}\eth\bar{\theta}$$

$$\eth\boldsymbol{q} = -\boldsymbol{\kappa}\cdot\eth\boldsymbol{\nabla}\boldsymbol{\theta}$$

The problem of homogenization

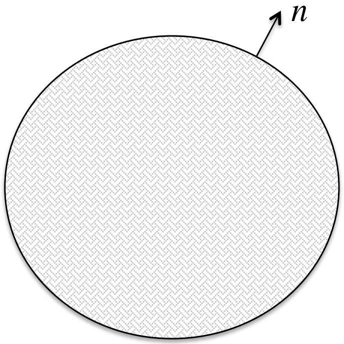
Given an heterogeneous material



Find an equivalent homogeneous material that has the same macroscopic behavior.

The problem of homogenization

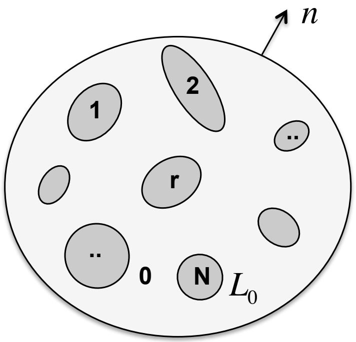
$$U_c = \frac{1}{2V}\int_V \sigma_{ij}\varepsilon_{ij}\, dV = \frac{1}{2}\overline{\sigma_{ij}\varepsilon_{ij}} \qquad U_h = \frac{1}{2}\bar{\sigma}_{ij}\bar{\varepsilon}_{ij}$$



Periodic media

Hill lemma:

$$\overline{\sigma_{ij}\varepsilon_{ij}} - \bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = \frac{1}{V}\int_S \left(u_i - x_j\bar{\varepsilon}_{ij}\right)\left(\sigma_{ik}n_k - \bar{\sigma}_{ik}n_k\right)\, dS$$



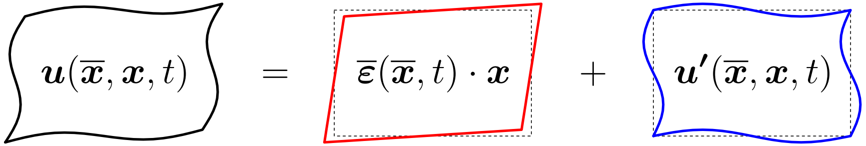
Random media

The Hill-Mandel theorem:

$$\overline{\sigma_{ij}\varepsilon_{ij}} - \bar{\sigma}_{ij}\bar{\varepsilon}_{ij} = 0$$

KUBC, SUBS, PBC

The problem of homogenization



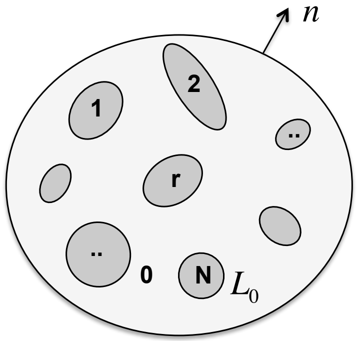
$$\boldsymbol{u}'(\overline{\boldsymbol{x}}, \boldsymbol{x}_+, t) = \boldsymbol{u}'(\overline{\boldsymbol{x}}, \boldsymbol{x}_-, t), \qquad \forall \overline{\boldsymbol{x}} \in \overline{V} \qquad \text{periodic}$$

$$\boldsymbol{\sigma}(\overline{\boldsymbol{x}}, \boldsymbol{x}_+, t) \cdot \boldsymbol{n}(\boldsymbol{x}_-) = -\boldsymbol{\sigma}(\overline{\boldsymbol{x}}, \boldsymbol{x}_+, t) \cdot \boldsymbol{n}(\boldsymbol{x}_+) \qquad \text{antiperiodic}$$

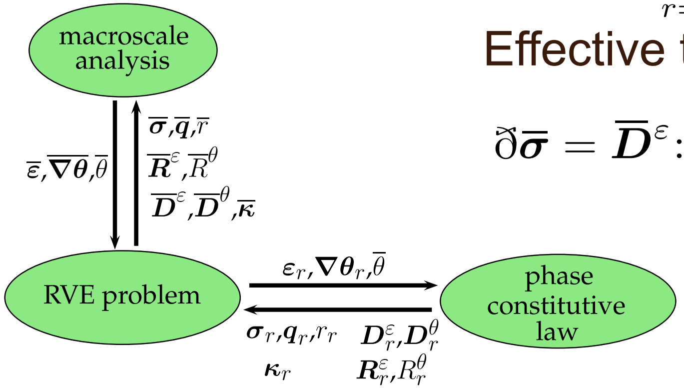
$$\begin{aligned}
\overline{\sigma_{ij}\varepsilon_{ij}} - \bar{\sigma}_{ij}\bar{\varepsilon}_{ij} &= \frac{1}{V}\int_V \boldsymbol{\sigma}(\overline{\boldsymbol{x}}, \boldsymbol{x}, t) : \boldsymbol{\varepsilon}(\overline{\boldsymbol{x}}, \boldsymbol{x}, t) \; dV - \overline{\boldsymbol{\sigma}}(\boldsymbol{x}, t) : \overline{\boldsymbol{\varepsilon}}(\boldsymbol{x}, t) \\
&= \frac{1}{V}\int_{\partial V} \Big(\boldsymbol{u}(\overline{\boldsymbol{x}}, \boldsymbol{x}, t) - \overline{\boldsymbol{\varepsilon}}(\overline{\boldsymbol{x}}, t) \cdot \boldsymbol{x}\Big) \cdot \Big(\boldsymbol{\sigma}(\overline{\boldsymbol{x}}, \boldsymbol{x}, t) \cdot \boldsymbol{n}(\boldsymbol{x}) - \overline{\boldsymbol{\sigma}}(\overline{\boldsymbol{x}}, t) \cdot \boldsymbol{n}(\boldsymbol{x})\Big) \; dS \\
&= \frac{1}{V}\int_{\partial V} \underbrace{\Big(\boldsymbol{u}'(\overline{\boldsymbol{x}}, \boldsymbol{x}, t) + \boldsymbol{u}_0(\overline{\boldsymbol{x}}, t)\Big)}_{\boldsymbol{u}' \quad \text{periodic}} \cdot \underbrace{\Big(\boldsymbol{\sigma}(\overline{\boldsymbol{x}}, \boldsymbol{x}, t) \cdot \boldsymbol{n}(\boldsymbol{x}) - \overline{\boldsymbol{\sigma}}(\overline{\boldsymbol{x}}, t) \cdot \boldsymbol{n}(\boldsymbol{x})\Big)}_{\boldsymbol{\sigma}\cdot\boldsymbol{n} \quad \text{anti-periodic}} \; dS = 0
\end{aligned}$$

➡ Non-linear : Linearized, incremental formulation

Non linear mean-field homogenization



Random media



Local thermoelastic increment

$$\Delta \boldsymbol{\varepsilon}_r = \boldsymbol{A}_r^{\varepsilon} : \Delta \overline{\boldsymbol{\varepsilon}} + \boldsymbol{A}_r^{\theta} \Delta \overline{\theta} \qquad \Delta \boldsymbol{\nabla}\boldsymbol{\theta}_r = \boldsymbol{A}_r^{\kappa} \cdot \Delta \overline{\boldsymbol{\nabla}\boldsymbol{\theta}}$$

Tangent quantities

$$\overline{\boldsymbol{D}}^{\varepsilon} = \sum_{r=0}^{N} f_r \boldsymbol{D}_r^{\varepsilon} : \boldsymbol{A}_r^{\varepsilon} \qquad \overline{\boldsymbol{D}}^{\theta} = \sum_{r=0}^{N} f_r \left[\boldsymbol{D}_r^{\theta} + \boldsymbol{D}_r^{\varepsilon} : \boldsymbol{A}_r^{\theta} \right] \qquad \overline{\boldsymbol{\kappa}} = \sum_{r=0}^{N} f_r \boldsymbol{\kappa}_r \cdot \boldsymbol{A}_r^{\kappa}$$

$$\overline{\boldsymbol{R}}^{\varepsilon} = \sum_{r=0}^{N} f_r \boldsymbol{R}_r^{\varepsilon} : \boldsymbol{A}_r^{\varepsilon} \qquad \overline{R}^{\theta} = \sum_{r=0}^{N} f_r \left[R_r^{\theta} + \boldsymbol{R}_r^{\varepsilon} : \boldsymbol{A}_r^{\theta} \right]$$

Effective thermoelastic law

$$\eth \overline{\boldsymbol{\sigma}} = \overline{\boldsymbol{D}}^{\varepsilon} : \eth \overline{\boldsymbol{\varepsilon}} + \overline{\boldsymbol{D}}^{\theta} \eth \overline{\theta} \qquad \eth \overline{\boldsymbol{q}} = -\overline{\boldsymbol{\kappa}} \cdot \eth \overline{\boldsymbol{\nabla}\boldsymbol{\theta}}$$

$$\eth \overline{r} = \overline{\boldsymbol{R}}^{\varepsilon} : \eth \overline{\boldsymbol{\varepsilon}} + \overline{R}^{\theta} \eth \overline{\theta}$$

Non-linear periodic homogenization

See Chatzigeorgiou et. al (2018)

Kinematics

$$\eth\boldsymbol{\varepsilon} = \eth\bar{\boldsymbol{\varepsilon}} + \mathrm{grad}_{\mathrm{sym}}\eth\widetilde{\boldsymbol{u}} \qquad \eth\boldsymbol{\nabla\theta} = \eth\overline{\boldsymbol{\nabla\theta}} + \mathrm{grad}\eth\widetilde{\theta}$$

Equilibrium

$$\mathrm{div}\left(\boldsymbol{D}^{\varepsilon}\!:\!\eth\bar{\boldsymbol{\varepsilon}} + \boldsymbol{D}^{\theta}\eth\bar{\theta} + \boldsymbol{D}^{\varepsilon}\!:\!\mathrm{grad}\eth\widetilde{\boldsymbol{u}}\right) = \boldsymbol{0}$$

$$\mathrm{div}\left(\boldsymbol{\kappa}\cdot\eth\overline{\boldsymbol{\nabla\theta}} + \boldsymbol{\kappa}\cdot\mathrm{grad}\eth\widetilde{\theta}\right) = 0$$

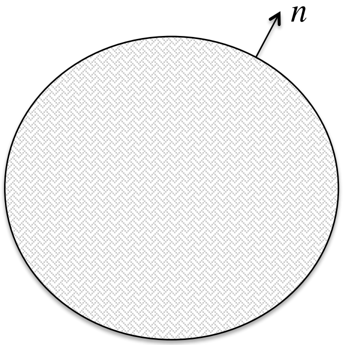
$$\eth\widetilde{\boldsymbol{u}} = \eth\bar{\boldsymbol{\varepsilon}}\!:\!\boldsymbol{\chi}^{\varepsilon} + \eth\bar{\theta}\;\boldsymbol{\chi}^{\theta}, \qquad \eth\widetilde{\theta} = \eth\overline{\boldsymbol{\nabla\theta}}\cdot\boldsymbol{\psi}^{\theta}$$

ENE H.I. (1983)

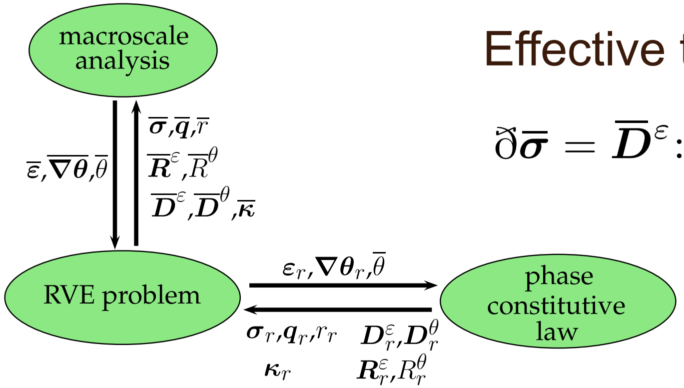
$$\eth\bar{\boldsymbol{\varepsilon}}\!:\!\mathrm{div}\left([\boldsymbol{D}^{\varepsilon} + \boldsymbol{D}^{\varepsilon}\,\tilde{:}\,\mathrm{grad}\boldsymbol{\chi}^{\varepsilon}]^{T}\right) + \eth\bar{\theta}\;\mathrm{div}\left(\boldsymbol{D}^{\theta} + \boldsymbol{D}^{\varepsilon}\!:\!\mathrm{grad}\boldsymbol{\chi}^{\theta}\right) = \boldsymbol{0} \qquad \mathrm{div}\left(\left[\boldsymbol{\kappa} + \boldsymbol{\kappa}\,\tilde{\cdot}\,\mathrm{grad}\boldsymbol{\psi}^{\theta}\right]^{T}\right) = \boldsymbol{0}$$

$$\mathrm{div}\left([\boldsymbol{D}^{\varepsilon} + \boldsymbol{D}^{\varepsilon}\,\tilde{:}\,\mathrm{grad}\boldsymbol{\chi}^{\varepsilon}]^{T}\right) = \boldsymbol{0} \qquad \eth\overline{\boldsymbol{\nabla\theta}}\cdot\mathrm{div}\left(\left[\boldsymbol{\kappa} + \boldsymbol{\kappa}\,\tilde{\cdot}\,\mathrm{grad}\boldsymbol{\psi}^{\theta}\right]^{T}\right) = \boldsymbol{0} \qquad \mathrm{div}\left(\boldsymbol{D}^{\theta} + \boldsymbol{D}^{\varepsilon}\!:\!\mathrm{grad}\boldsymbol{\chi}^{\theta}\right) = \boldsymbol{0}$$

Non-linear periodic homogenization



Periodic media



Local thermoelastic increment

$$\Delta\boldsymbol{\varepsilon}_r = \boldsymbol{A}^{\varepsilon}_r : \Delta\bar{\boldsymbol{\varepsilon}} + \boldsymbol{A}^{\theta}_r \Delta\bar{\theta} \qquad \Delta\boldsymbol{\nabla\theta}_r = \boldsymbol{A}^{\kappa}_r \cdot \Delta\overline{\boldsymbol{\nabla\theta}}$$

Tangent quantities

$$\overline{\boldsymbol{D}}^{\varepsilon} = \langle \boldsymbol{D}^{\varepsilon} : \boldsymbol{A}^{\varepsilon} \rangle \qquad \overline{\boldsymbol{D}}^{\theta} = \left\langle \boldsymbol{D}^{\theta} + \boldsymbol{D}^{\varepsilon} : \boldsymbol{A}^{\theta} \right\rangle \qquad \bar{\boldsymbol{\kappa}} = \langle \boldsymbol{\kappa} \cdot \boldsymbol{A}^{\kappa} \rangle$$

$$\overline{\boldsymbol{R}}^{\varepsilon} = \langle \boldsymbol{R}^{\varepsilon} : \boldsymbol{A}^{\varepsilon} \rangle \qquad \overline{R}^{\theta} = \left\langle R^{\theta} + \boldsymbol{R}^{\varepsilon} : \boldsymbol{A}^{\theta} \right\rangle$$

$$\boldsymbol{A}^{\varepsilon} = \boldsymbol{\mathcal{I}} + \boldsymbol{\mathcal{I}} \,\tilde{:}\, \mathrm{grad}\boldsymbol{\chi}^{\varepsilon}$$

Effective thermoelastic law

$$\eth\bar{\boldsymbol{\sigma}} = \overline{\boldsymbol{D}}^{\varepsilon} : \eth\bar{\boldsymbol{\varepsilon}} + \overline{\boldsymbol{D}}^{\theta} \eth\bar{\theta} \qquad \eth\bar{\boldsymbol{q}} = -\bar{\boldsymbol{\kappa}} \cdot \eth\overline{\boldsymbol{\nabla\theta}}$$

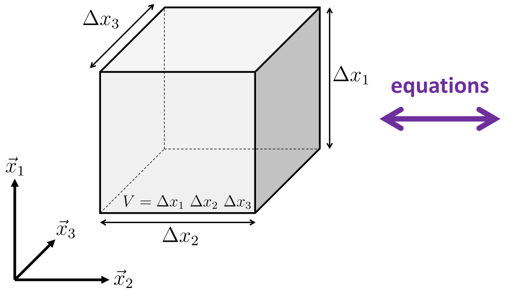
$$\boldsymbol{A}^{\theta} = \mathrm{grad}_{\mathrm{sym}}\boldsymbol{\chi}^{\theta}$$

$$\eth\bar{r} = \overline{\boldsymbol{R}}^{\varepsilon} : \eth\bar{\boldsymbol{\varepsilon}} + \overline{R}^{\theta} \eth\bar{\theta} \qquad \boldsymbol{A}^{\kappa} = \boldsymbol{I} + \left[\mathrm{grad}\boldsymbol{\psi}^{\theta}\right]^{T}$$

FE² (Among other multiscale models)

Suquet periodic homogenization solution

$$\begin{Bmatrix} u_1^i - u_1^j \\ u_2^i - u_2^j \\ u_3^i - u_3^j \end{Bmatrix} = \begin{pmatrix} \overline{\varepsilon}_{11} & \overline{\varepsilon}_{12} & \overline{\varepsilon}_{13} \\ & \overline{\varepsilon}_{22} & \overline{\varepsilon}_{23} \\ \text{sym.} & & \overline{\varepsilon}_{33} \end{pmatrix} \times \begin{Bmatrix} x_1^i - x_1^j \\ x_2^i - x_2^j \\ x_3^i - x_3^j \end{Bmatrix}$$



- $u_{11}^{cd} = \overline{\varepsilon}_{11} \quad \Leftrightarrow \quad F_{11}^{cd} = \overline{\sigma}_{11} V$
- $u_{22}^{cd} = \overline{\varepsilon}_{22} \quad \Leftrightarrow \quad F_{22}^{cd} = \overline{\sigma}_{22} V$
- $u_{33}^{cd} = \overline{\varepsilon}_{33} \quad \Leftrightarrow \quad F_{33}^{cd} = \overline{\sigma}_{33} V$
- $u_{12}^{cd} = 2\overline{\varepsilon}_{12} \quad \Leftrightarrow \quad F_{12}^{cd} = \overline{\sigma}_{12} V$
- $u_{13}^{cd} = 2\overline{\varepsilon}_{13} \quad \Leftrightarrow \quad F_{13}^{cd} = \overline{\sigma}_{13} V$
- $u_{23}^{cd} = 2\overline{\varepsilon}_{23} \quad \Leftrightarrow \quad F_{23}^{cd} = \overline{\sigma}_{23} V$

Figure I.5: Connection of the "constraint drivers" with the unit cell

$$\begin{cases} \Delta\overline{\boldsymbol{\varepsilon}}_{(11)} = (K \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)^T \\ \Delta\overline{\boldsymbol{\varepsilon}}_{(22)} = (0 \quad K \quad 0 \quad 0 \quad 0 \quad 0)^T \\ \Delta\overline{\boldsymbol{\varepsilon}}_{(33)} = (0 \quad 0 \quad K \quad 0 \quad 0 \quad 0)^T \\ \Delta\overline{\boldsymbol{\varepsilon}}_{(12)} = (0 \quad 0 \quad 0 \quad K \quad 0 \quad 0)^T \\ \Delta\overline{\boldsymbol{\varepsilon}}_{(13)} = (0 \quad 0 \quad 0 \quad 0 \quad K \quad 0)^T \\ \Delta\overline{\boldsymbol{\varepsilon}}_{(23)} = (0 \quad 0 \quad 0 \quad 0 \quad 0 \quad K)^T \end{cases}$$

$$\begin{Bmatrix} \Delta\overline{\sigma}_{11} \\ \Delta\overline{\sigma}_{22} \\ \Delta\overline{\sigma}_{33} \\ \Delta\overline{\sigma}_{12} \\ \Delta\overline{\sigma}_{13} \\ \Delta\overline{\sigma}_{23} \end{Bmatrix} = \begin{pmatrix} \overline{D}_{1111}^{\varepsilon} & \overline{D}_{1122}^{\varepsilon} & \overline{D}_{1133}^{\varepsilon} & \overline{D}_{1112}^{\varepsilon} & \overline{D}_{1113}^{\varepsilon} & \overline{D}_{1123}^{\varepsilon} \\ & \overline{D}_{2222}^{\varepsilon} & \overline{D}_{2233}^{\varepsilon} & \overline{D}_{2212}^{\varepsilon} & \overline{D}_{2213}^{\varepsilon} & \overline{D}_{2223}^{\varepsilon} \\ & & \overline{D}_{3333}^{\varepsilon} & \overline{D}_{3312}^{\varepsilon} & \overline{D}_{3313}^{\varepsilon} & \overline{D}_{3323}^{\varepsilon} \\ & & & \overline{D}_{1212}^{\varepsilon} & \overline{D}_{1213}^{\varepsilon} & \overline{D}_{1223}^{\varepsilon} \\ & & & & \overline{D}_{1313}^{\varepsilon} & \overline{D}_{1323}^{\varepsilon} \\ Sym & & & & & \overline{D}_{2323}^{\varepsilon} \end{pmatrix} \times \begin{Bmatrix} \Delta\overline{\varepsilon}_{11} \\ \Delta\overline{\varepsilon}_{22} \\ \Delta\overline{\varepsilon}_{33} \\ 2\,\Delta\overline{\varepsilon}_{12} \\ 2\,\Delta\overline{\varepsilon}_{13} \\ 2\,\Delta\overline{\varepsilon}_{23} \end{Bmatrix}$$

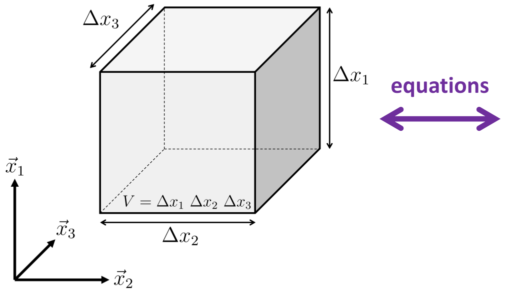
$$\overline{D}_{ijkl}^{\varepsilon} = \frac{\Delta\overline{\boldsymbol{\sigma}}_{ij(kl)}}{K}, \qquad ij, kl = 11, 22, 33, 12, 13, 23$$

Tikarrouchine, Ph.D. dissertation (2019)

FE² (Among other multiscale models)

Suquet periodic homogenization solution

$$\begin{Bmatrix} u_1^i - u_1^j \\ u_2^i - u_2^j \\ u_3^i - u_3^j \end{Bmatrix} = \begin{pmatrix} \overline{\varepsilon}_{11} & \overline{\varepsilon}_{12} & \overline{\varepsilon}_{13} \\ & \overline{\varepsilon}_{22} & \overline{\varepsilon}_{23} \\ \text{sym.} & & \overline{\varepsilon}_{33} \end{pmatrix} \times \begin{Bmatrix} x_1^i - x_1^j \\ x_2^i - x_2^j \\ x_3^i - x_3^j \end{Bmatrix}$$



- $u_{11}^{cd} = \overline{\varepsilon}_{11} \Leftrightarrow F_{11}^{cd} = \overline{\sigma}_{11} V$
- $u_{22}^{cd} = \overline{\varepsilon}_{22} \Leftrightarrow F_{22}^{cd} = \overline{\sigma}_{22} V$
- $u_{33}^{cd} = \overline{\varepsilon}_{33} \Leftrightarrow F_{33}^{cd} = \overline{\sigma}_{33} V$
- $u_{12}^{cd} = 2\overline{\varepsilon}_{12} \Leftrightarrow F_{12}^{cd} = \overline{\sigma}_{12} V$
- $u_{13}^{cd} = 2\overline{\varepsilon}_{13} \Leftrightarrow F_{13}^{cd} = \overline{\sigma}_{13} V$
- $u_{23}^{cd} = 2\overline{\varepsilon}_{23} \Leftrightarrow F_{23}^{cd} = \overline{\sigma}_{23} V$

Figure I.5: Connection of the "constraint drivers" with the unit cell

$$\begin{Bmatrix} \Delta\overline{\sigma}_{11} \\ \Delta\overline{\sigma}_{22} \\ \Delta\overline{\sigma}_{33} \\ \Delta\overline{\sigma}_{12} \\ \Delta\overline{\sigma}_{13} \\ \Delta\overline{\sigma}_{23} \end{Bmatrix} = \begin{pmatrix} \overline{D}^{\varepsilon}_{1111} & \overline{D}^{\varepsilon}_{1122} & \overline{D}^{\varepsilon}_{1133} & \overline{D}^{\varepsilon}_{1112} & \overline{D}^{\varepsilon}_{1113} & \overline{D}^{\varepsilon}_{1123} \\ & \overline{D}^{\varepsilon}_{2222} & \overline{D}^{\varepsilon}_{2233} & \overline{D}^{\varepsilon}_{2212} & \overline{D}^{\varepsilon}_{2213} & \overline{D}^{\varepsilon}_{2223} \\ & & \overline{D}^{\varepsilon}_{3333} & \overline{D}^{\varepsilon}_{3312} & \overline{D}^{\varepsilon}_{3313} & \overline{D}^{\varepsilon}_{3323} \\ & & & \overline{D}^{\varepsilon}_{1212} & \overline{D}^{\varepsilon}_{1213} & \overline{D}^{\varepsilon}_{1223} \\ & & & & \overline{D}^{\varepsilon}_{1313} & \overline{D}^{\varepsilon}_{1323} \\ Sym & & & & & \overline{D}^{\varepsilon}_{2323} \end{pmatrix} \times \begin{Bmatrix} \Delta\overline{\varepsilon}_{11} \\ \Delta\overline{\varepsilon}_{22} \\ \Delta\overline{\varepsilon}_{33} \\ 2\,\Delta\overline{\varepsilon}_{12} \\ 2\,\Delta\overline{\varepsilon}_{13} \\ 2\,\Delta\overline{\varepsilon}_{23} \end{Bmatrix}$$

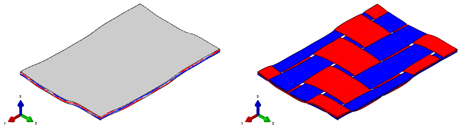

(a) Entire unit cell (b) Yarns

Figure I.11: Deflection of the unit cell for the unitary strain state $\overline{\varepsilon}_{(11)}$.

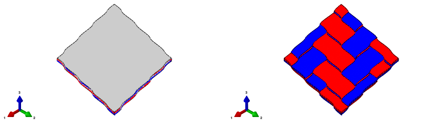

(a) Entire unit cell (b) Yarns

Figure I.14: Deflection of the unit cell for the unitary strain state $\overline{\varepsilon}_{(12)}$.

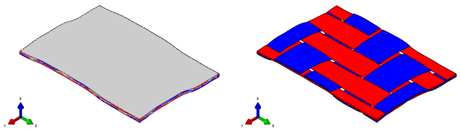

(a) Entire unit cell (b) Yarns

Figure I.12: Deflection of the unit cell for the unitary strain state $\overline{\varepsilon}_{(22)}$.

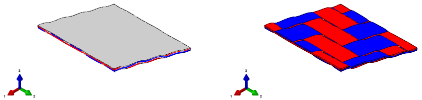

(a) Entire unit cell (b) Yarns

Figure I.15: Deflection of the unit cell for the unitary strain state $\overline{\varepsilon}_{(13)}$.

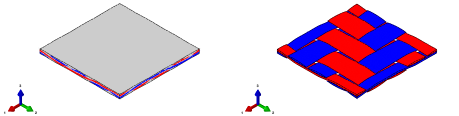

(a) Entire unit cell (b) Yarns

Figure I.13: Deflection of the unit cell for the unitary strain state $\overline{\varepsilon}_{(33)}$.

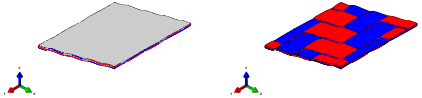
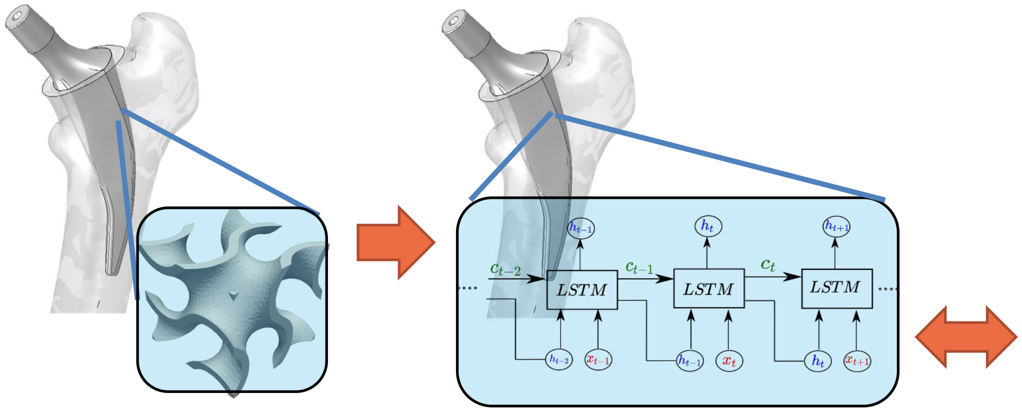
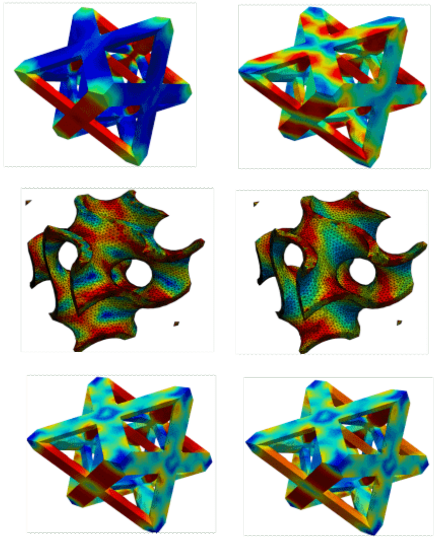

(a) Entire unit cell (b) Yarns

Figure I.16: Deflection of the unit cell for the unitary strain state $\overline{\varepsilon}_{(23)}$.

Praud, Ph.D. dissertation (2018)

Motivation : Can we significantly speed up?





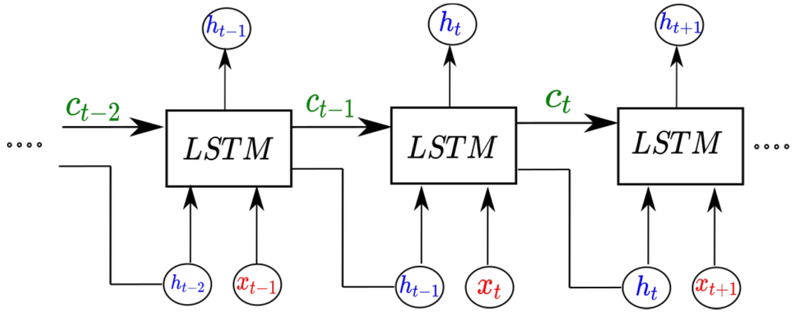
Offline database

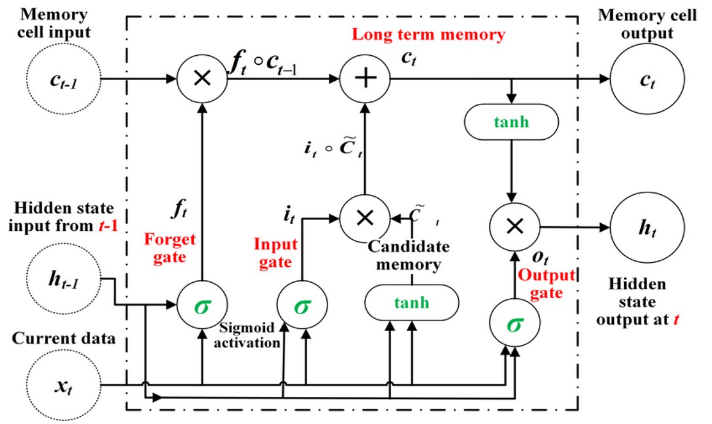
Replace FE^2 with AI models:

- Adapted for constitutive models with internal variables (memory/microstructural evolution)
- FE convergence ? Implementation in FE solutions ?
- Estimated speedup factor ~ 10000 (Settgast et al.2019). To be checked for NP loadings / real cases

History = Recurrent Neural Network

Long-short term memory



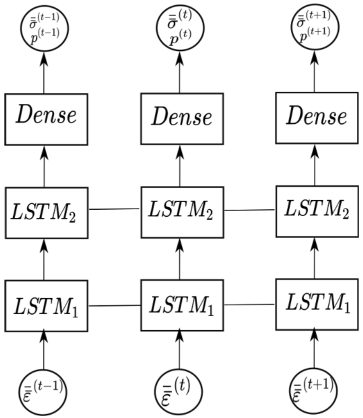


- $x_t \in \mathbb{R}^d$: input vector to the LSTM unit
- $f_t \in \mathbb{R}^h$: forget gate's activation vector
- $i_t \in \mathbb{R}^h$: input/update gate's activation vector
- $o_t \in \mathbb{R}^h$: output gate's activation vector
- $h_t \in \mathbb{R}^h$: hidden state vector also known as output vector of the LSTM unit
- $\tilde{c}_t \in \mathbb{R}^h$: cell input activation vector
- $c_t \in \mathbb{R}^h$: cell state vector
- $W \in \mathbb{R}^{h \times d}$, $U \in \mathbb{R}^{h \times h}$ and $b \in \mathbb{R}^h$: weight matrices and bias vector parameters which need to be learned during training

$$
\begin{aligned}
f_t &= \sigma_g(W_f x_t + U_f h_{t-1} + b_f) \\
i_t &= \sigma_g(W_i x_t + U_i h_{t-1} + b_i) \\
o_t &= \sigma_g(W_o x_t + U_o h_{t-1} + b_o) \\
\tilde{c}_t &= \tanh(W_c x_t + U_c h_{t-1} + b_c) \\
c_t &= f_t \circ c_{t-1} + i_t \circ \tilde{c}_t \\
h_t &= o_t \circ \tanh(c_t)
\end{aligned}
$$

History = Recurrent Neural Network

$$\Delta x^{(n+1)(m+1)(k+1)} = \Delta x^{(n+1)(m+1)(k)} + \delta x^{(n+1)(m+1)(k)}$$



Chosen RNN architecture

Model's inputs : Incremental Strain tensor components

Model's outputs : Incremental Stress tensor components + internal variables (if any)

Mechanical properties of titanium alloy Ti-6Al-4V

Material parameter	**Value**
Young's modulus E	113800 MPa
Poisson's ratio ν	0.34
Yield Stress σ_Y	1000 MPa
Hardening parameter H	1600 MPa
Plastic hardening exponent n	0.5

Example 1 : Power-law hardening

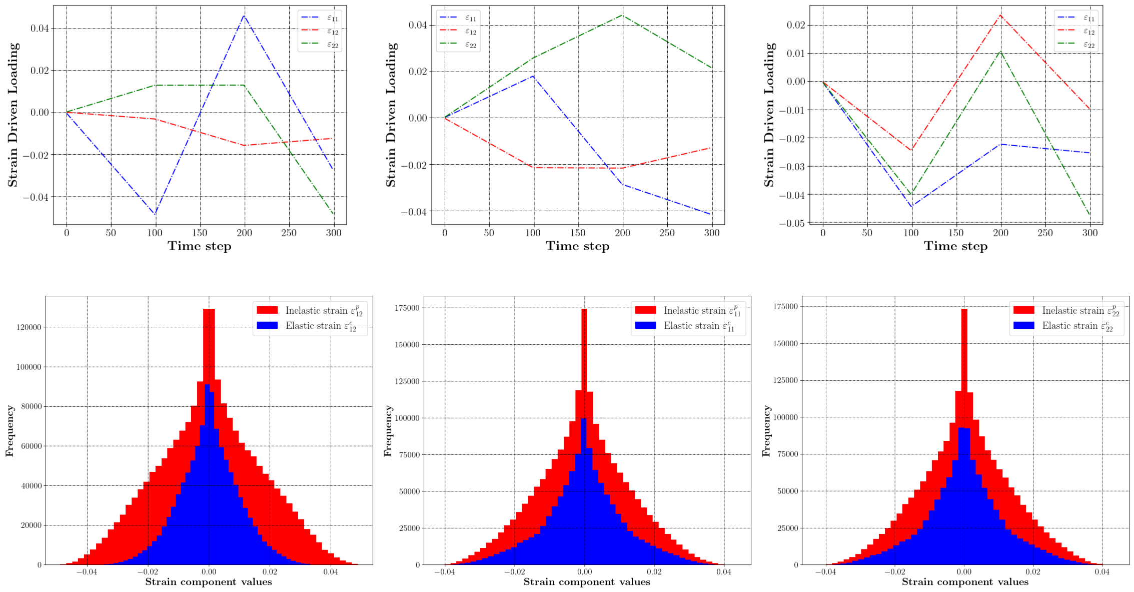
Training

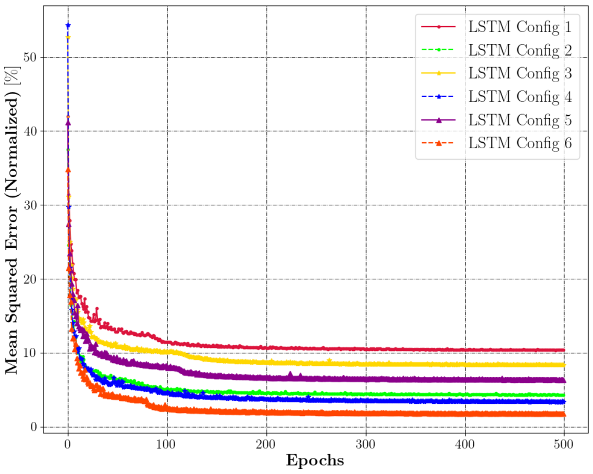
Classical Mean Squared Error (MSE)

$$\mathcal{L}_t = \frac{1}{N}\sum^{N}\left(y_t^{(p)} - y_t^{(true)}\right)^2$$

Mean Squared Error (MSE) with thermodynamic constraint

$$\mathcal{L}_t^{\varphi} = \frac{1}{N}\sum^{N}(y_t^{(p)} - y_t^{(true)})^2 + \lambda Relu(-\gamma_{loc})$$





Danoun et. al (2022)

Training

Classical Mean Squared Error (MSE)

$$\mathcal{L}_t = \frac{1}{N}\sum^{N}\left(y_t^{(p)} - y_t^{(true)}\right)^2$$

Mean Squared Error (MSE) with thermodynamic constraint

$$\mathcal{L}_t^{\varphi} = \frac{1}{N}\sum^{N}(y_t^{(p)} - y_t^{(true)})^2 + \lambda Relu(-\gamma_{loc})$$

Non-linear homogenization .. Difficulty to relate $\eth\gamma_{\text{loc}}$ to the stress increment

$$\eth\gamma_{\text{loc}} = \boldsymbol{\Gamma}^{\varepsilon}:\eth\boldsymbol{\varepsilon} + \Gamma^{\theta}\eth\bar{\theta}$$

Work to do here

Model – Chaboche with 2 NL kinematical hardenings

$$\Psi^{\text{r}}\left(\varepsilon, \varepsilon^{\text{p}}, \boldsymbol{a_1}, \boldsymbol{a_2}\right) = \frac{1}{2}\left[\varepsilon - \varepsilon^{\text{p}}\right] : \boldsymbol{L} : \left[\varepsilon - \varepsilon^{\text{p}}\right] + \frac{1}{3}C_1\boldsymbol{a_1} : \boldsymbol{a_1} + \frac{1}{3}C_2\boldsymbol{a_2} : \boldsymbol{a_2}$$

$$\Psi^{\text{ir}}(p) = H(p)$$

$$\dot{\boldsymbol{X}}_{\boldsymbol{1}} = \frac{2}{3}C_1\dot{\varepsilon}^p - D_1\boldsymbol{X_1}\dot{p}$$

$$\dot{\boldsymbol{X}}_{\boldsymbol{2}} = \frac{2}{3}C_2\dot{\varepsilon}^p - D_2\boldsymbol{X_1}\dot{p}$$

$$\dot{H} = b(Q - H)\dot{p}$$

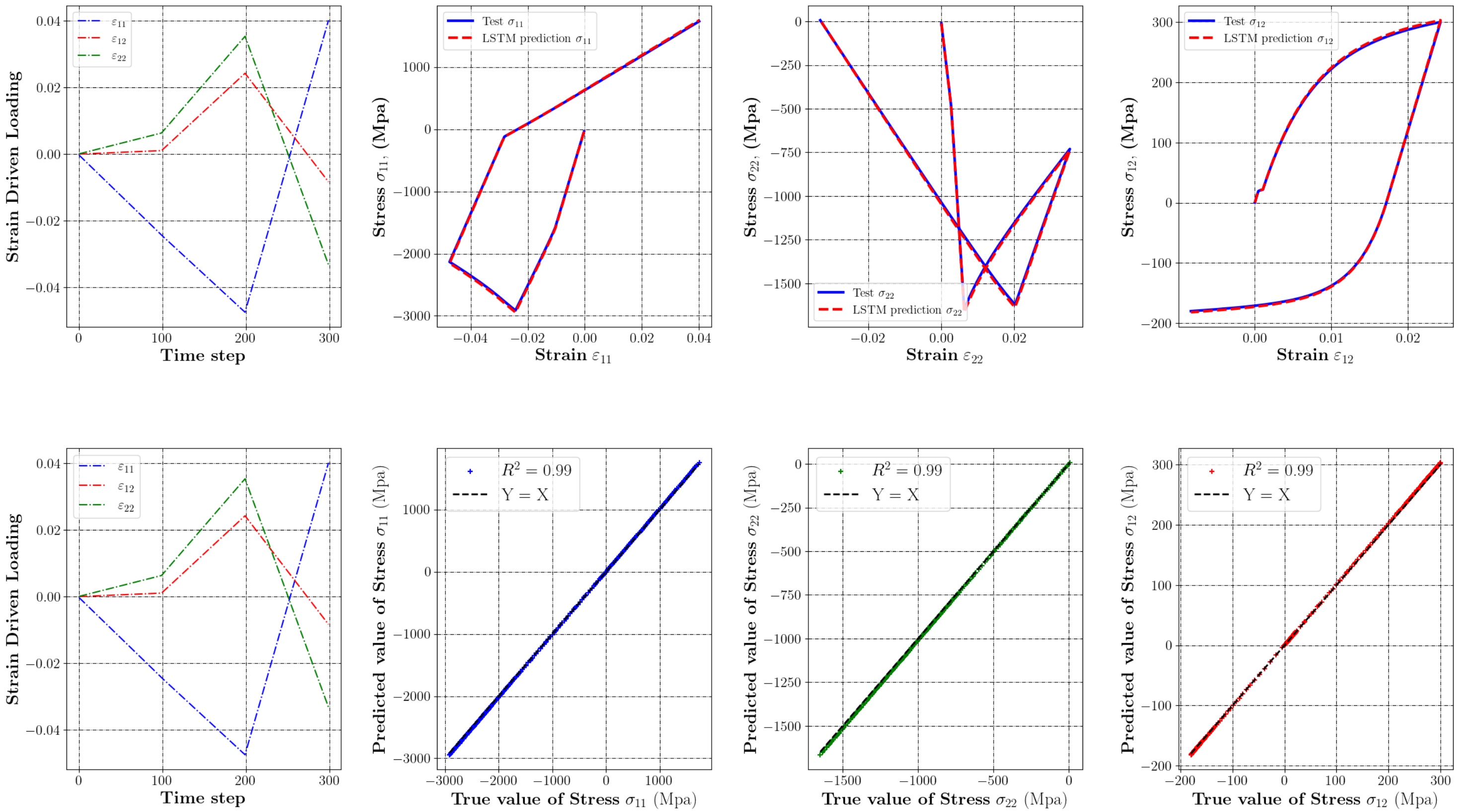
$$\dot{\text{W}}_{\text{m}}^{\text{r}} = \sigma : \left[\dot{\varepsilon} - \dot{\varepsilon}^{\text{P}}\right] + \boldsymbol{X_1} : \dot{a}_1 + \boldsymbol{X_2} : \dot{a}_2$$

$$\dot{\text{W}}_{\text{m}}^{\text{ir}} = \frac{\partial H}{\partial p}\dot{p}$$

$$\gamma_{\text{loc}} = -\frac{\partial\Psi^{\text{r}}}{\partial\varepsilon^{\text{p}}} : \dot{\varepsilon}^{\text{p}} - \frac{\partial\Psi^{\text{r}}}{\partial a_1} : \dot{a}_1 - \frac{\partial\Psi^{\text{r}}}{\partial a_2} : \dot{a}_2 - \frac{\partial\Psi^{\text{ir}}}{\partial p}\dot{p}$$

$$\gamma_{\text{loc}} = \boldsymbol{\sigma} : \dot{\varepsilon}^{\text{p}} - \boldsymbol{X_1} : \dot{\boldsymbol{a}}_{\boldsymbol{1}} - \boldsymbol{X_2} : \dot{\boldsymbol{a}}_{\boldsymbol{2}} - \frac{\partial H}{\partial p}\dot{p}.$$

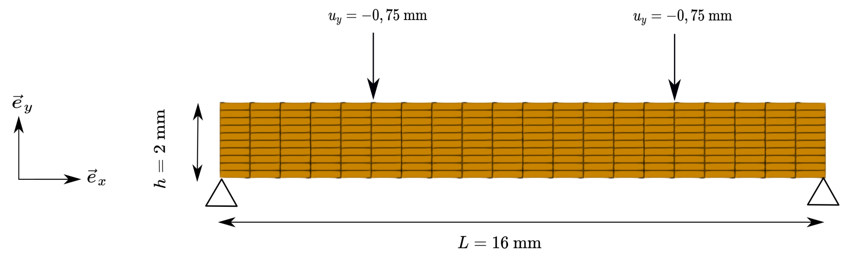
Validation with thermodynamics consistent training

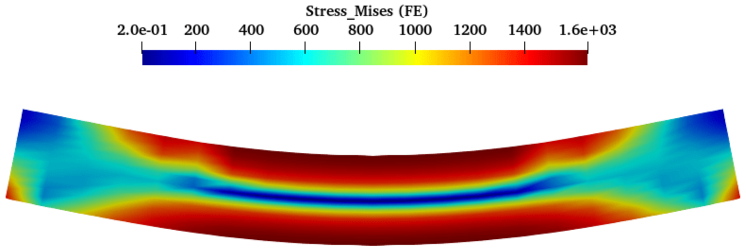


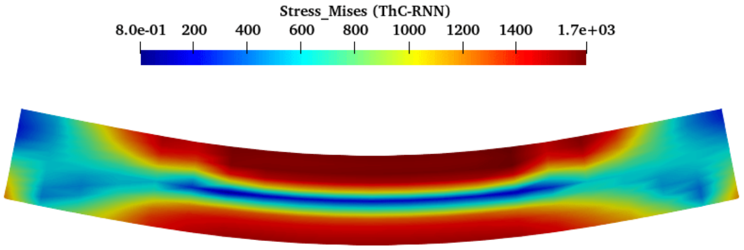
Danoun et. al (2022)

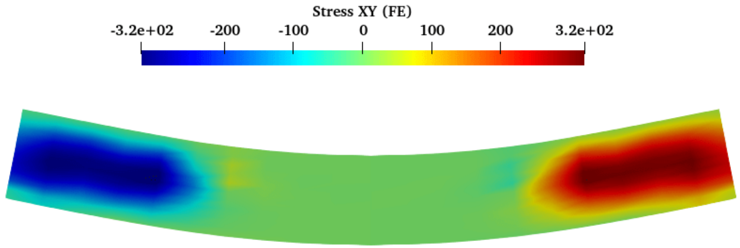
Structure validation

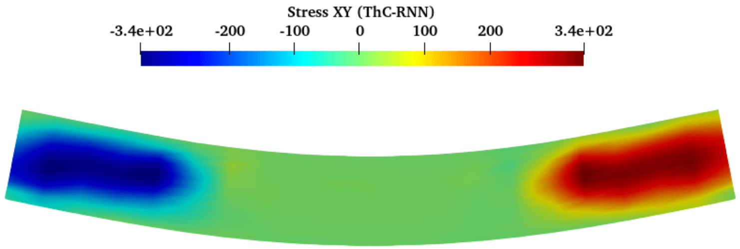
Similar convergence rates!







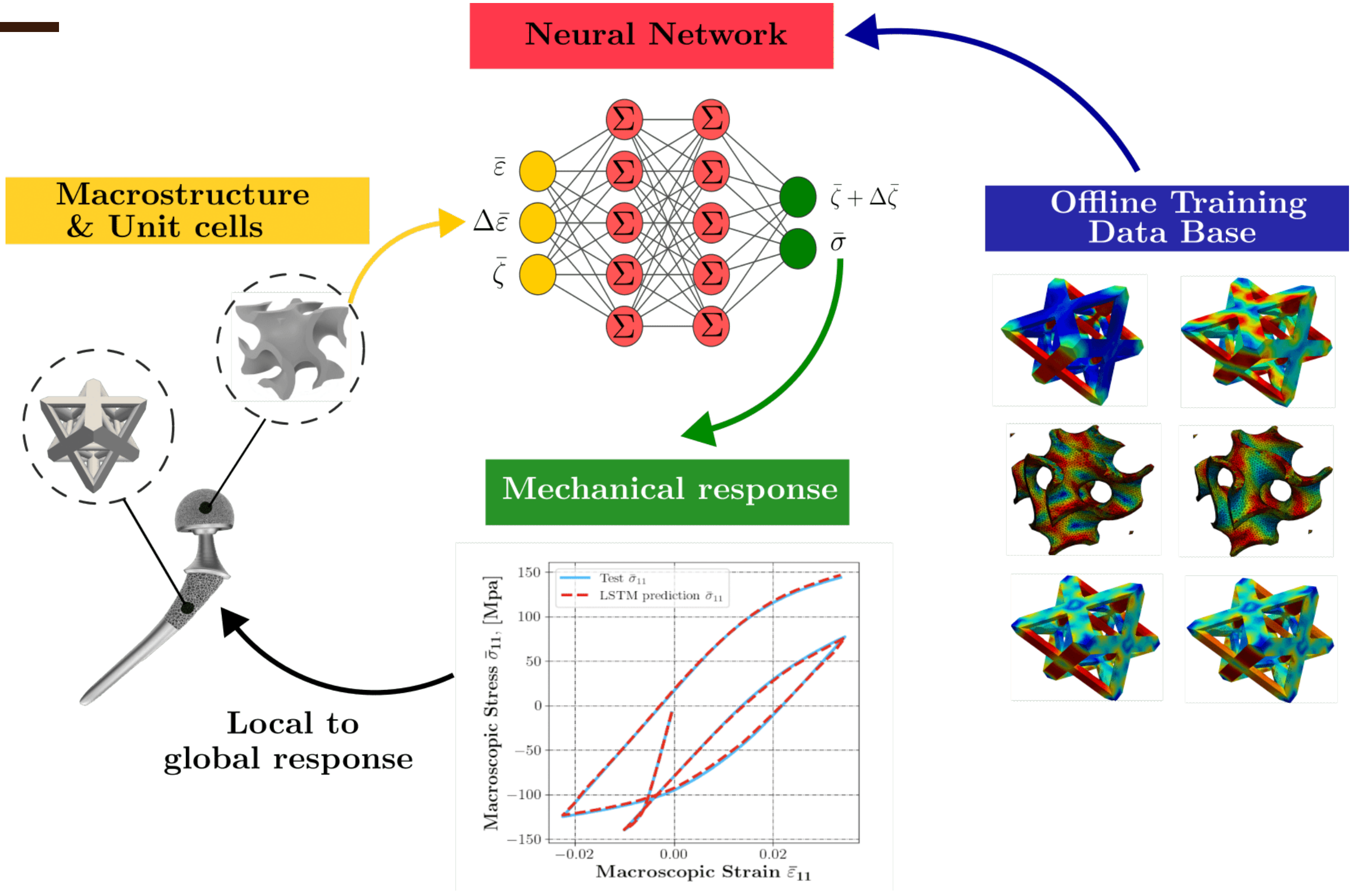




Constitutive model (original)

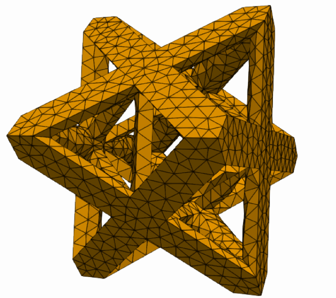
ThC RNN

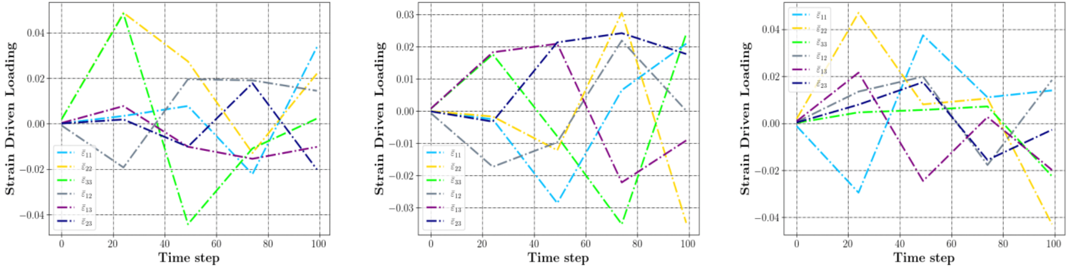
Multiscale simulations

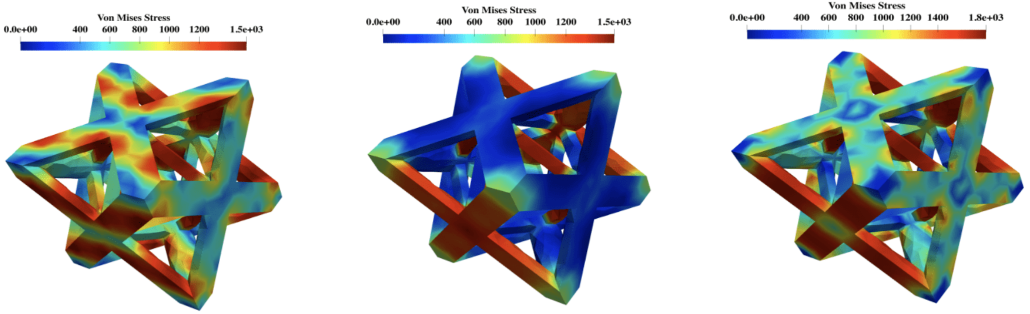


Database

Material parameter	Value
Young's modulus E	113800 MPa
Poisson's ratio ν	0.34
Yield Stress σ_Y	1000 MPa
Hardening parameter H	1600 Mpa
Plastic hardening exponent n	0.5
External cylinders radius R_e	0.1
Internal cylinders radius R_i	0.05







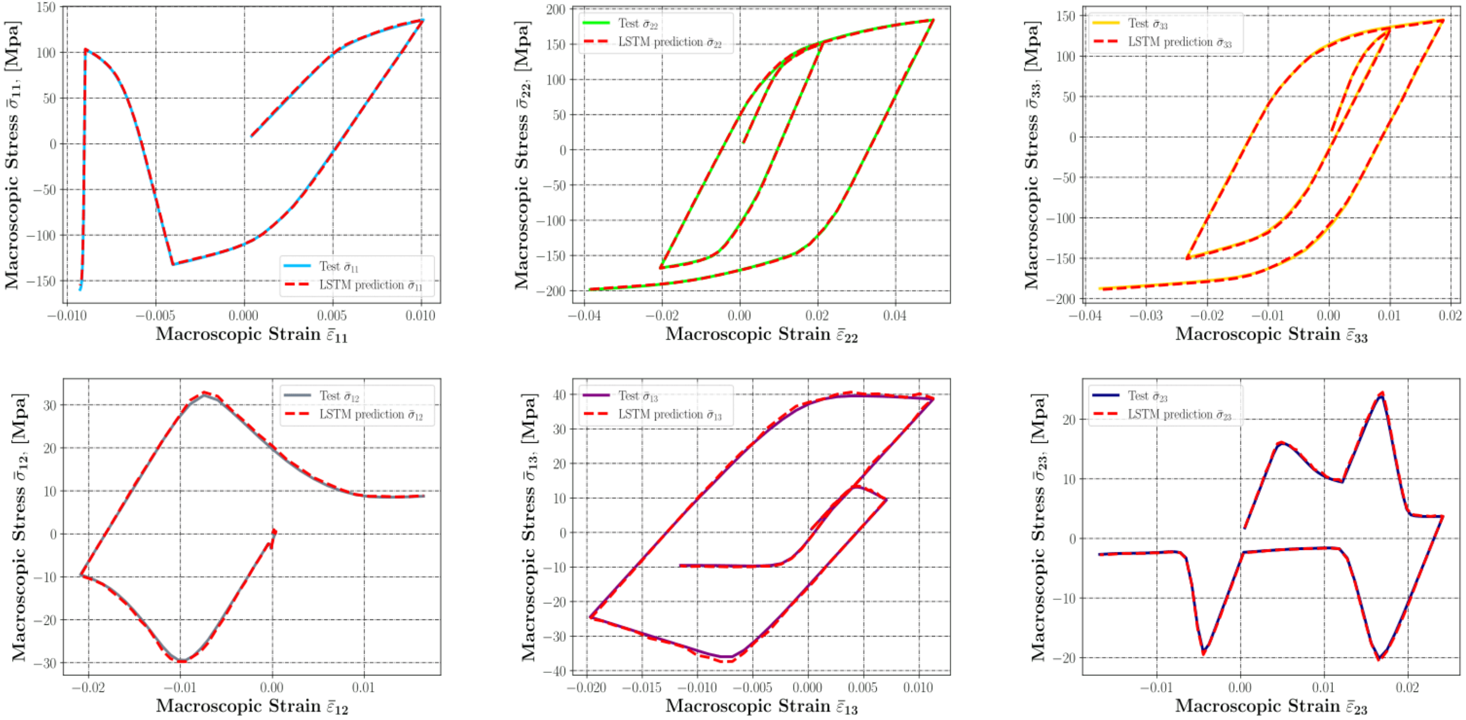
10000 simulations:
90% training
10% validation

Important features
- Non-proportional loadings
- Random path in strain space
- Database =

Updated stress
Tangent modulus
Mechanical power

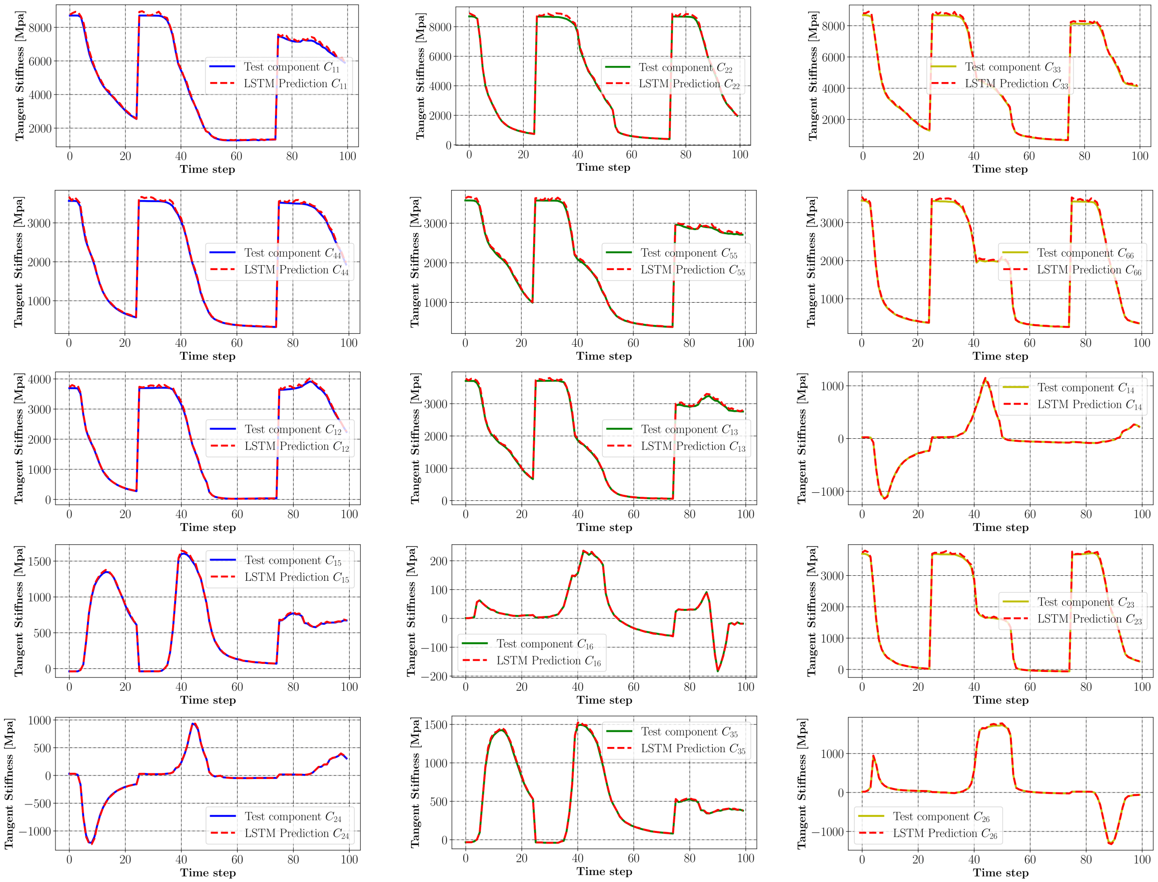
Danoun et. al (2024)

Macroscopic stress response



Danoun et. al (2024)

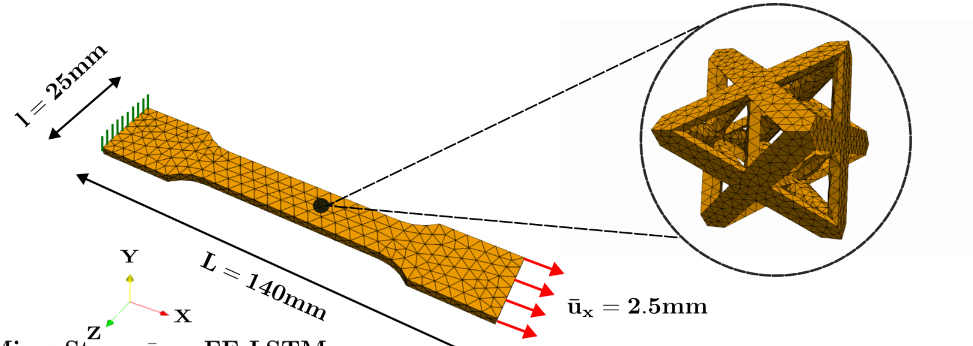
Tangent modulus



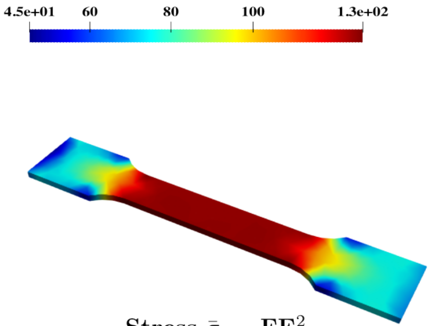
Second LSTM network to predict the tangent modulus

Danoun et. al (2024)

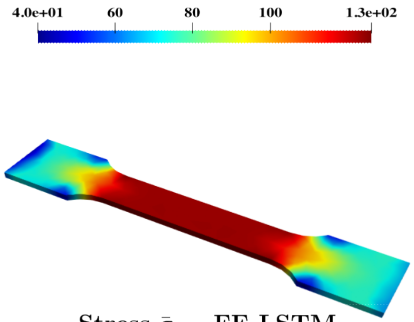
Multiscale structures



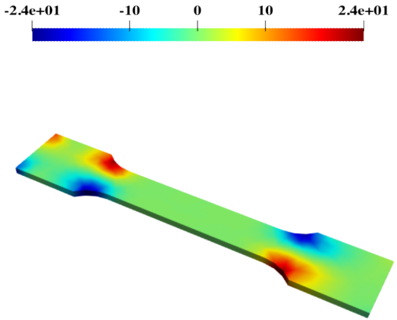
Von Mises Stress $\bar{\sigma}_{VM}$ FE^2



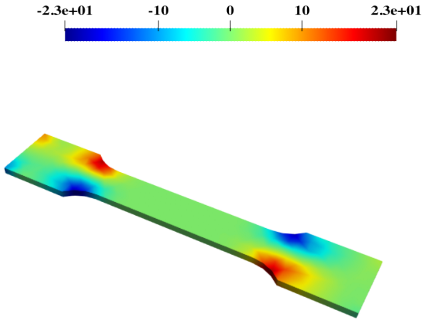
Von Mises Stress $\bar{\sigma}_{VM}$ FE-LSTM



Stress $\bar{\sigma}_{XZ}$ FE^2



Stress $\bar{\sigma}_{XZ}$ FE-LSTM



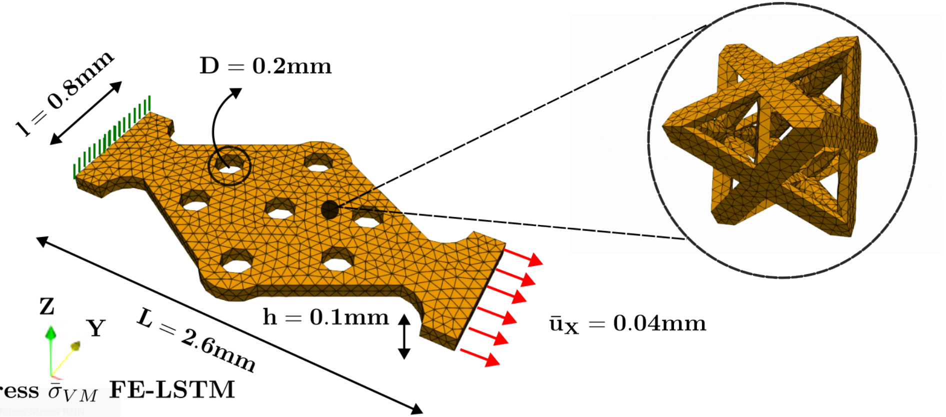
Macroscopic stress components

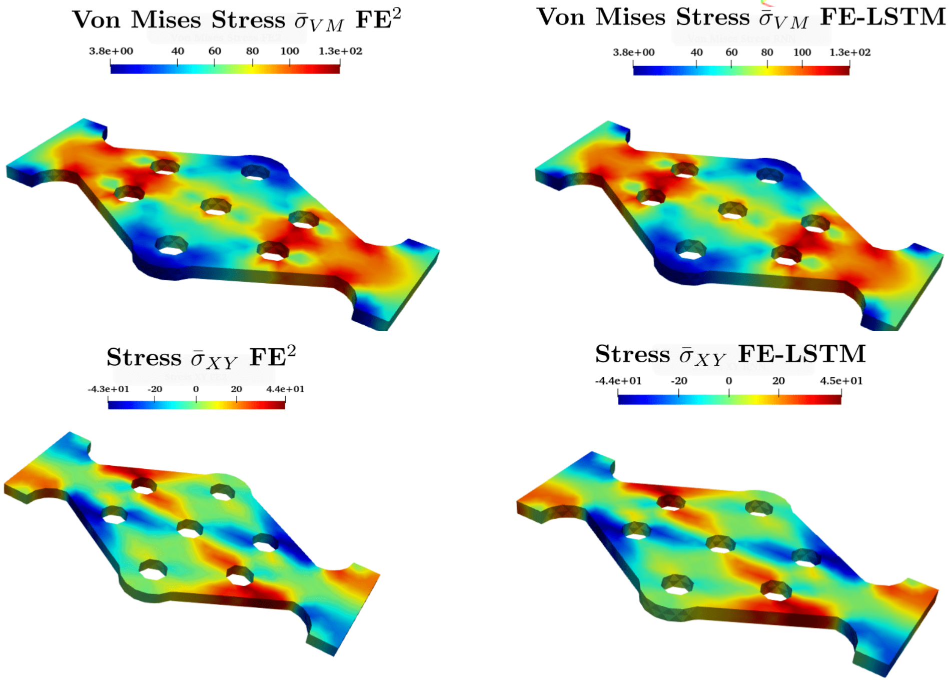
MAPE (%)

Stress $\bar{\sigma}_{VM}$	Stress $\bar{\sigma}_{XX}$
0.02 %	0.01 %
Stress $\bar{\sigma}_{ZZ}$	Stress $\bar{\sigma}_{XZ}$
2.04 %	0.44 %

Average normalized error

Multiscale structures





Macroscopic stress components

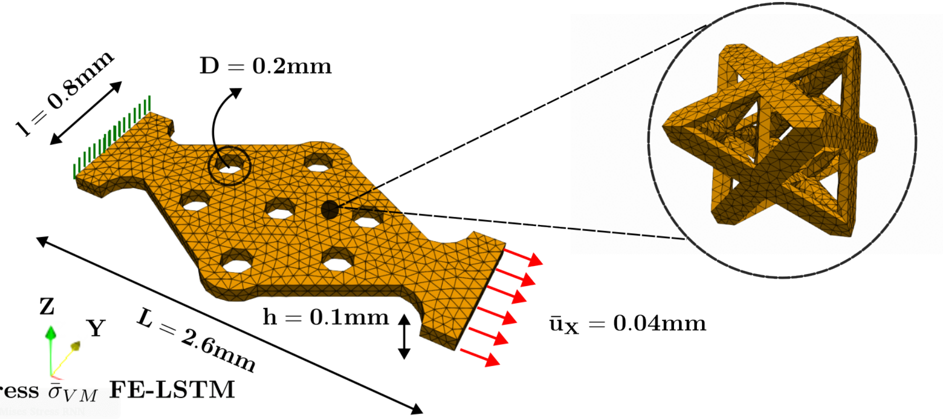
MAPE (%)

Stress $\bar{\sigma}_{VM}$	Stress $\bar{\sigma}_{XX}$
0.03 %	0.03 %

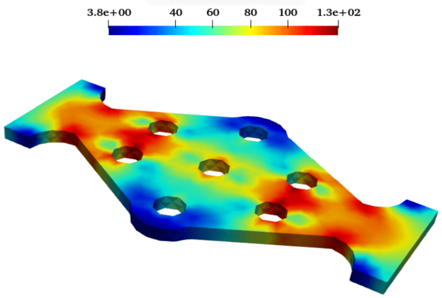
Stress $\bar{\sigma}_{ZZ}$	Stress $\bar{\sigma}_{XZ}$
1.58 %	1.97 %

Average normalized error

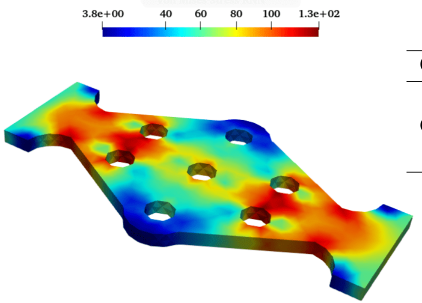
Multiscale structures



Von Mises Stress $\bar{\sigma}_{VM}$ FE^2



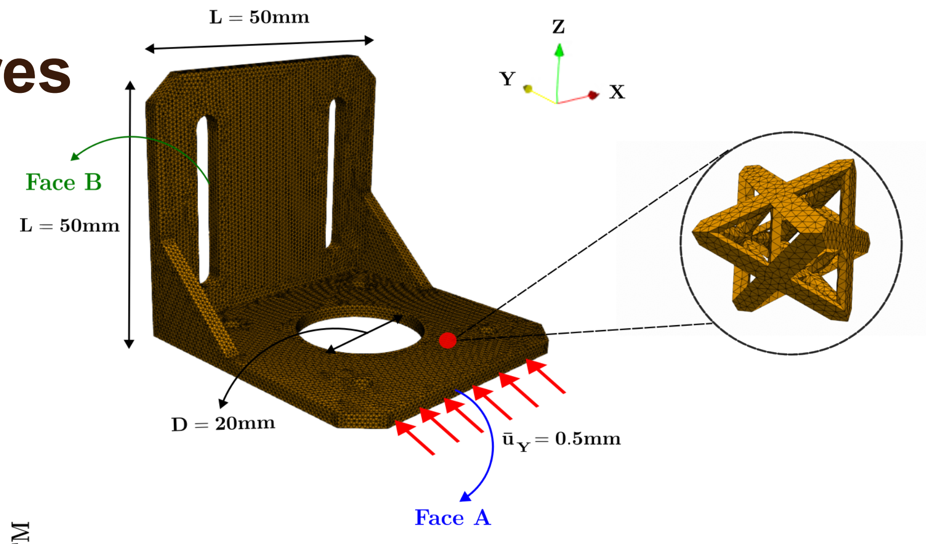
Von Mises Stress $\bar{\sigma}_{VM}$ FE-LSTM

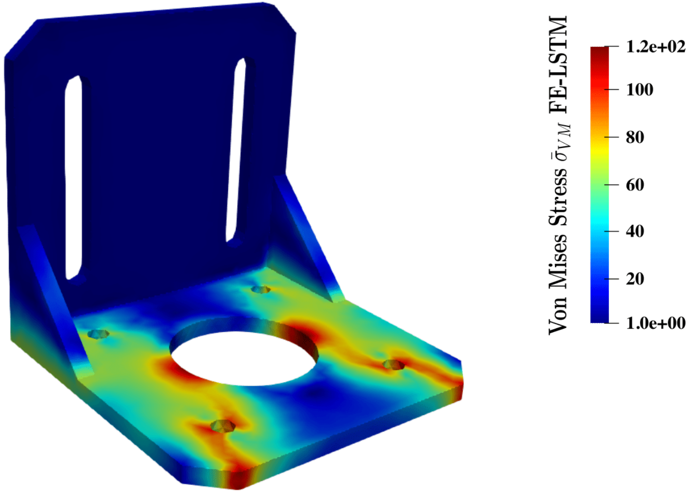


Offline computations	**Database generation**	**LSTM training**
Computational time	70 hours	5.5 hours

	FE^2 simulation	**FE-LSTM simulation**	**Computational time saving factor**	**Memory usage saving factor**
Online simulation time	5 days	102 seconds	4235	–
Memory usage	1.07 TB	120 MB	–	8917

Multiscale structures





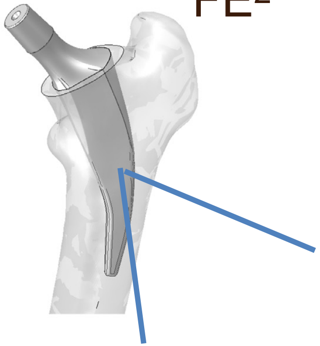
Not possible with FE^2:

Estimated RAM : 22.84 TB
Estimated comp time (1 CPU) 105 days

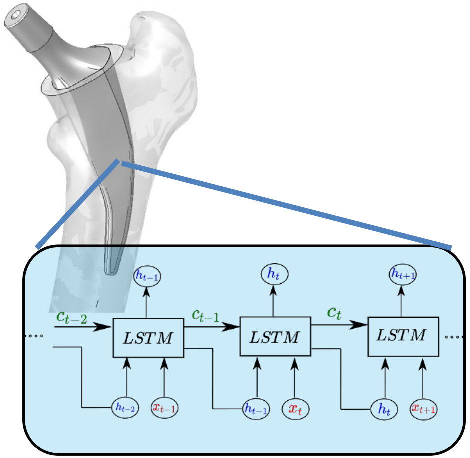
FE – RNN :
RAM : 2.5 GB
Comp time : 35 min

Conclusions

FE^2



FE + IA



Easy to implement : NOT intrusive

Extension to time-dependent reponse : TO DO

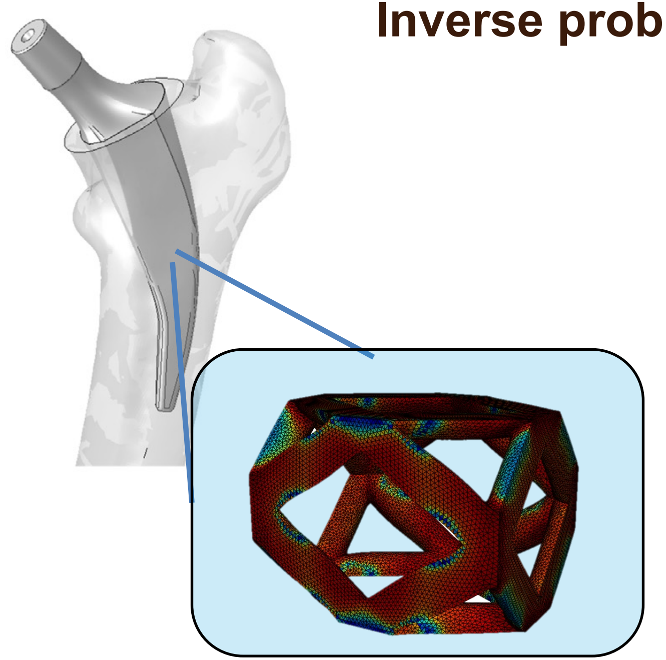
Extension to finite transformation : TO DO

Estimated speedup factor ~ 1000 – 40000x

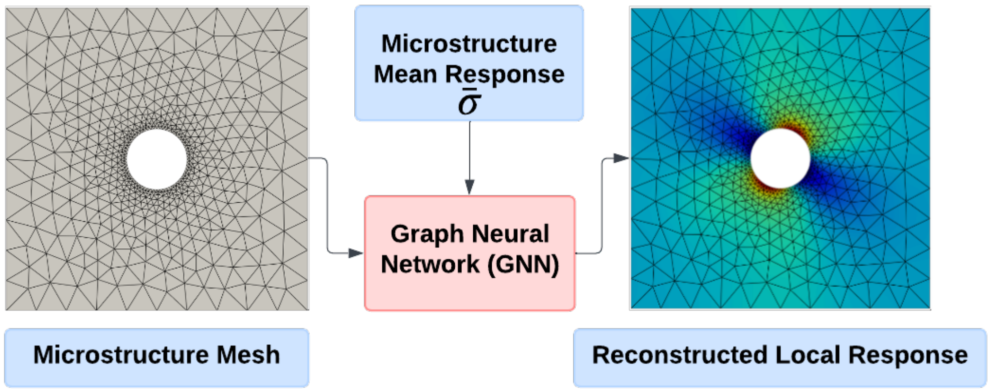
Challenges : Varying microstructure ⇨ Computer Vision

Local fields ⇨ Field reconstruction

Localization problems



Inverse problems, we want to predict local fields

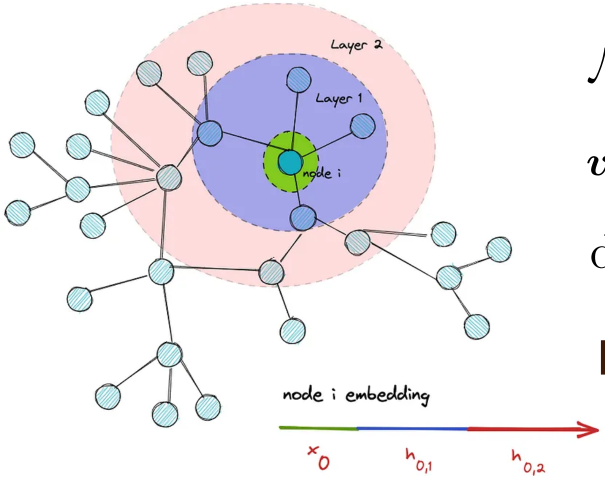


Can IA help of should we rely on full-field simulations?

Obtain local fields from a FE simulation using an effective model

Ph.D. Guevara Garban (in progress)

Use of graph Neural Network



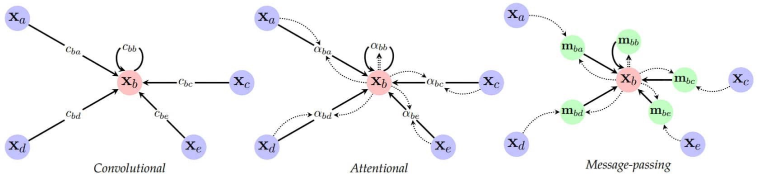
$\mathcal{M} = (\mathcal{V}, \mathcal{E})$ is an undirected graph

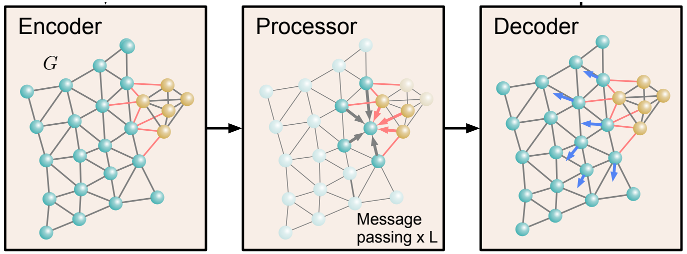
$\boldsymbol{v}_i = (\bar{\sigma}, p_i, \alpha_i)$ is a node feature node vector,

$\mathrm{dist}(p_j, p_i)$ Euclidian distance for feature edge

Periodicity : 0 euclidian distance for « pair » nodes

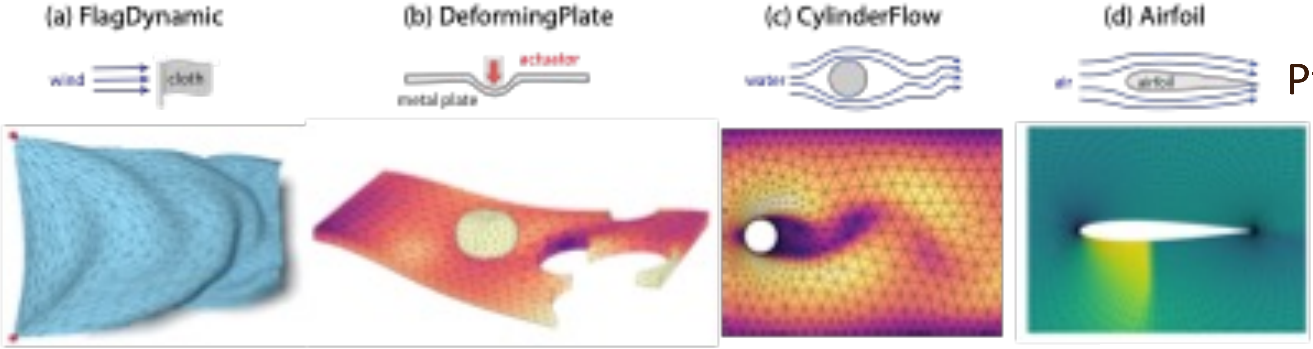
Encode –Message Passing - Decode model:





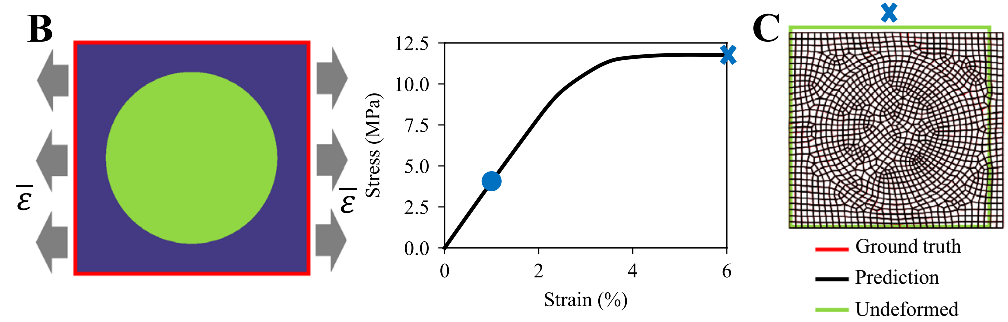
Message Passing using an MLP

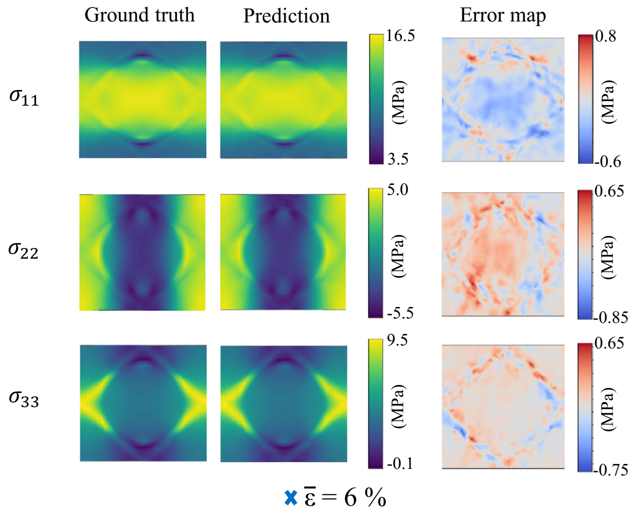
Use of meshGraphNet in mechanics



Pfaff, M. et al (ICLR), 2021.

M. Maurizi, Scientific Reports 12 (2022).





Under the hood

Encode –Message Passing - Decode model:

$$\mathrm{GNN}(\boldsymbol{v}_i, \mathcal{M}) \mapsto (\hat{\sigma}_{xx_i}, \hat{\sigma}_{yy_i}, \hat{\sigma}_{xy_i})$$

Features Local stress field

1 - Encode

$$\boldsymbol{v}_i' = \epsilon^V(\boldsymbol{v}_i), \quad \boldsymbol{e}_{ij}' = \epsilon^E(\boldsymbol{e}_{ij}) \quad \boldsymbol{v}_i' \in \mathbb{R}^H \text{ and } \boldsymbol{e}_{ij}' \in \mathbb{R}^H$$

2 – Message passing

$$\mathcal{M}' = (\mathcal{V}', \mathcal{E}')$$

$$\boldsymbol{e}_{ij}'' = \phi^{(l)}(\boldsymbol{v}_i', \boldsymbol{v}_j', \boldsymbol{e}_{ij}') \qquad \boldsymbol{e}_{ij}'' \in \mathbb{R}^H$$

$$\boldsymbol{v}_i'' = \gamma^{(l)}\left(\boldsymbol{v}_i', \sum_{j \in \mathcal{N}(i)} \boldsymbol{e}_{ij}''\right) \qquad \boldsymbol{v}_i'' \in \mathbb{R}^H$$

Repeat L times

3 – Decode

$$\mathcal{M}'' = (\mathcal{V}'', \mathcal{E}'')$$

$$\delta^V(\boldsymbol{v}_i'') \mapsto \boldsymbol{o}_i \qquad \boldsymbol{o}_i \in \mathbb{R}^O$$

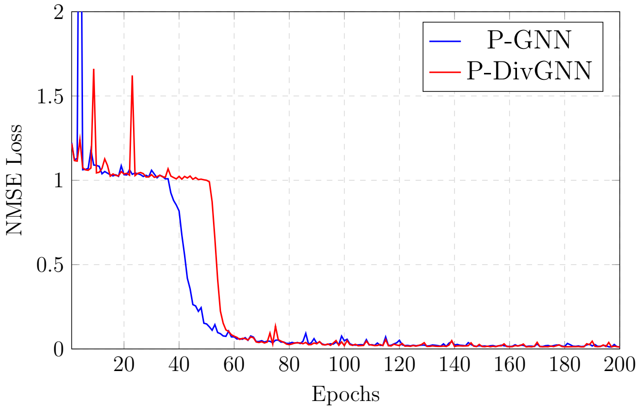
MLP acting on node features processed in the latent space to get $(\hat{\sigma}_{xx_i}, \hat{\sigma}_{yy_i}, \hat{\sigma}_{xy_i})$

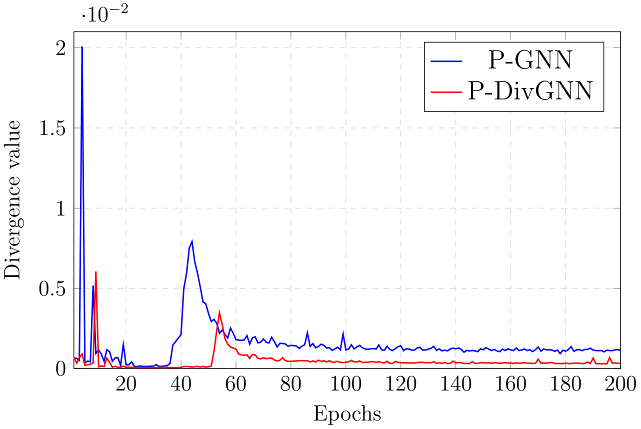
Adding physics?:

$$\mathcal{L}(\sigma, \hat{\sigma}) = \text{NMSE}(\sigma, \hat{\sigma}) + \lambda\left(\textbf{div}(\hat{\boldsymbol{\sigma}})\right)^2$$

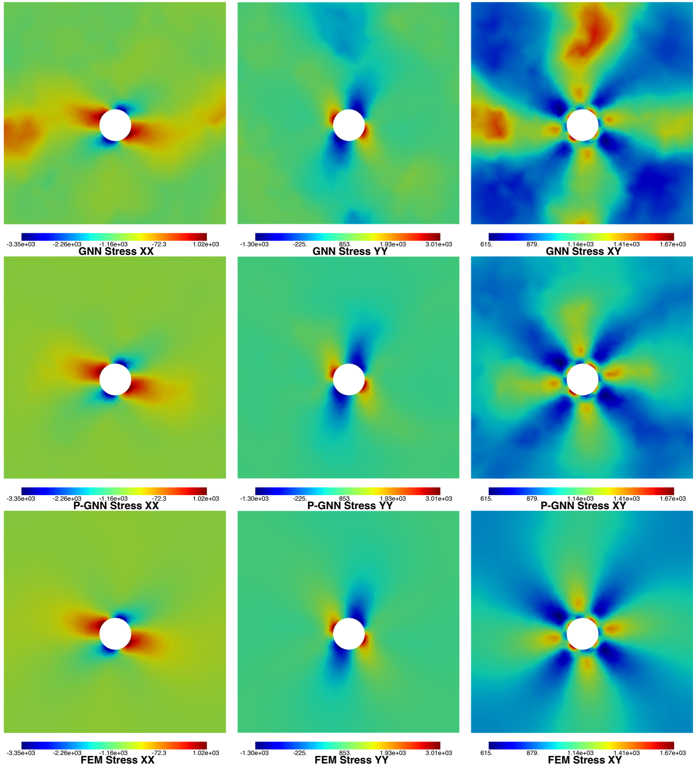
$$\text{NMSE}(\sigma, \hat{\sigma}) = \frac{1}{N_c}\sum_{c=1}^{N_c}\frac{\sum_{i=1}^{N}(\sigma_{c,i}-\hat{\sigma}_{c,i})^2}{\sum_{i=1}^{N}(\sigma_{c,i}-\frac{1}{N}\sum_{j=1}^{N}\sigma_{c,j})^2}$$

$$\left(\textbf{div}(\hat{\boldsymbol{\sigma}})\right)^2 = \frac{1}{N}\sum_{i=1}^{N}\left[(\textbf{div}(\hat{\boldsymbol{\sigma}})_i)_1^2 + (\textbf{div}(\hat{\boldsymbol{\sigma}})_i)_2^2\right]$$

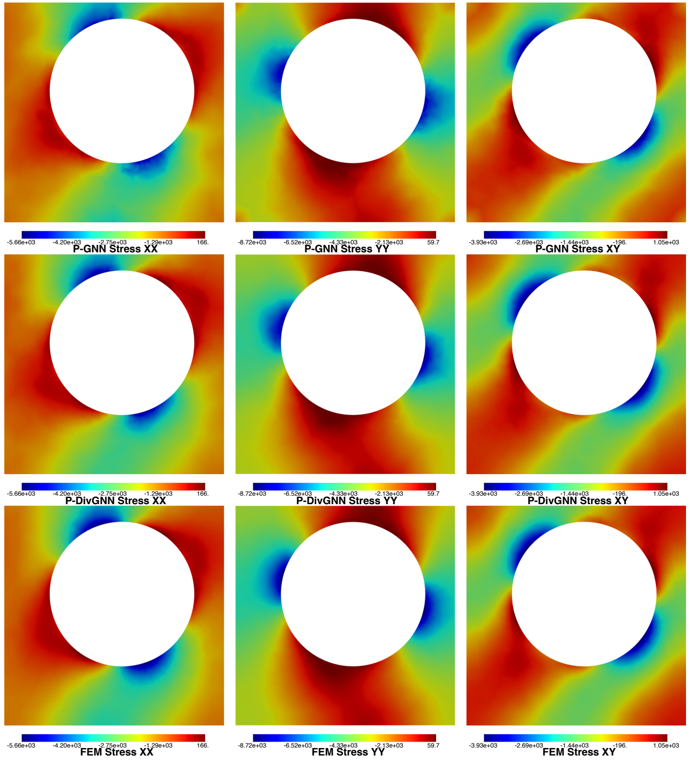




Results



Local stress reconstruction comparison between classical GNN (without periodic edges) in top row, *P-GNN* in middle row, and *FEM* in bottom row.



Local stress reconstruction comparison between *P-GNN*, *P-DivGNN* models and *FEM* the color bar scale is set using the FE solution ranges

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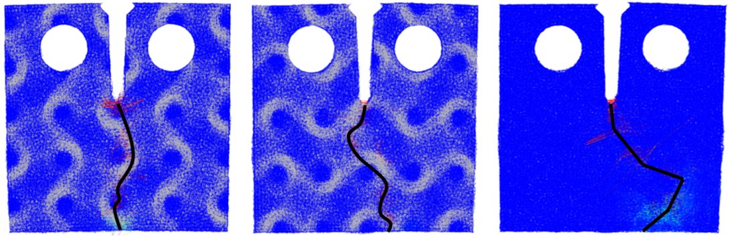
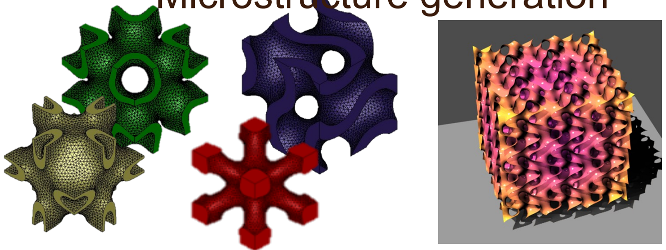
granoo

Discrete Element Method



microgen

Microstructure generation



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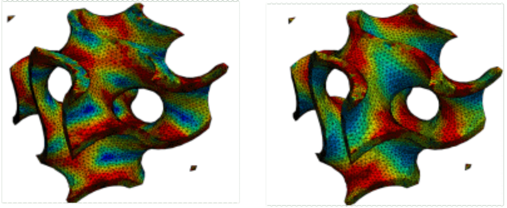
Finite Element library for multiscale analysis, Model reduction



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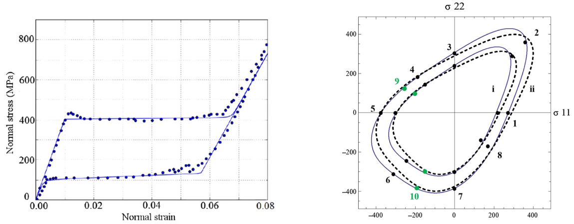
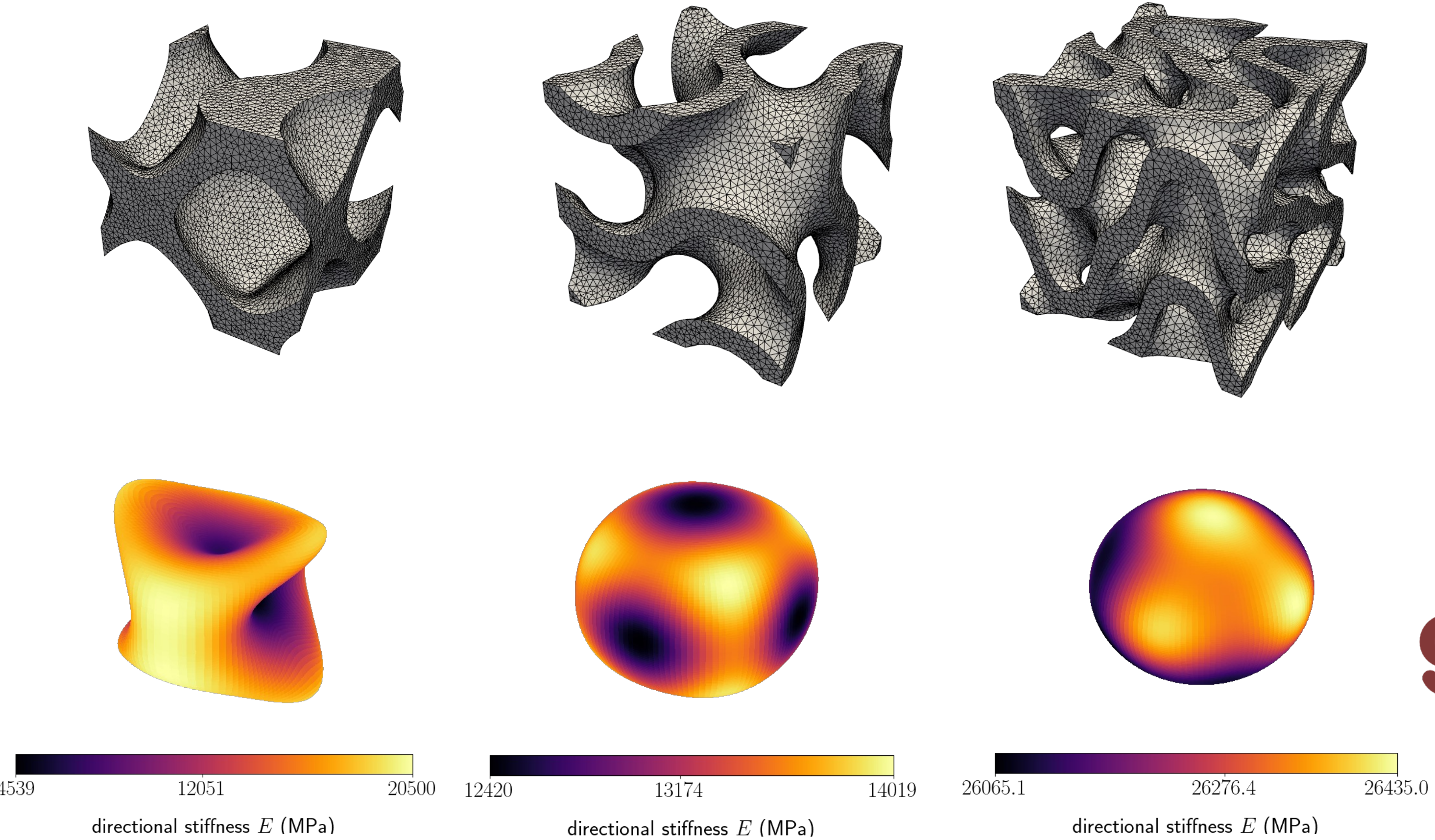
Material constitutive laws





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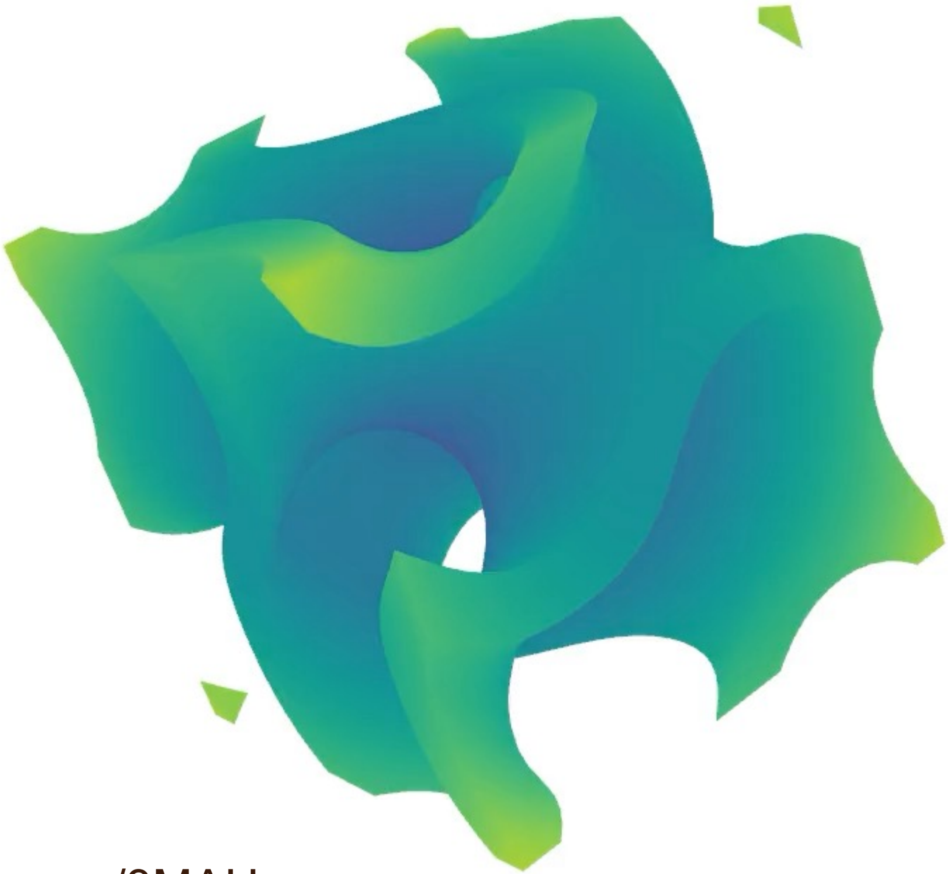

https://github.com/3MAH

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