Deep Material Networks

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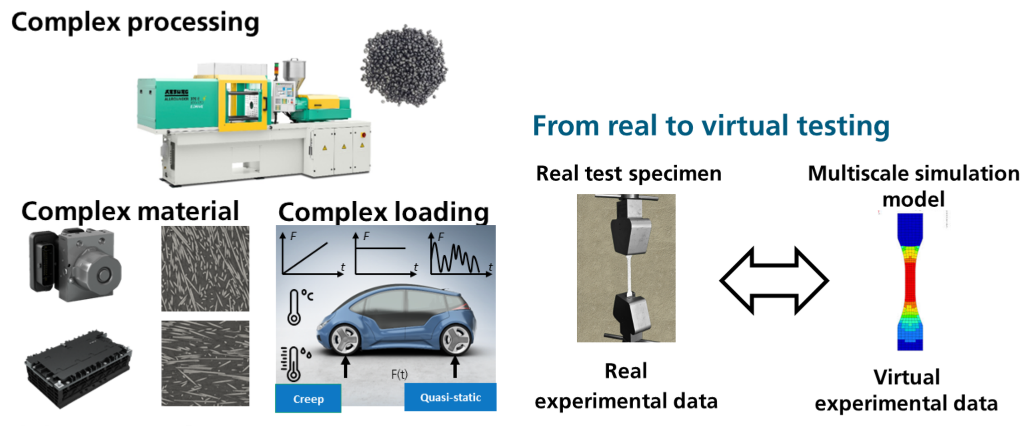
Motivation

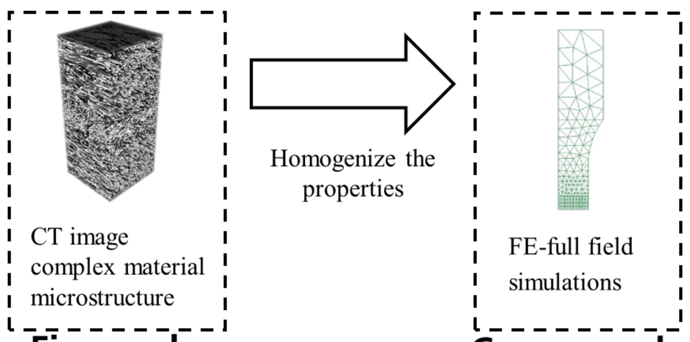
Reliability despite complexity



Problem Real experiments ≡ expensive & sparse.
Strategy: Calibrated multiscale simulations ⇒ virtual experimental data.

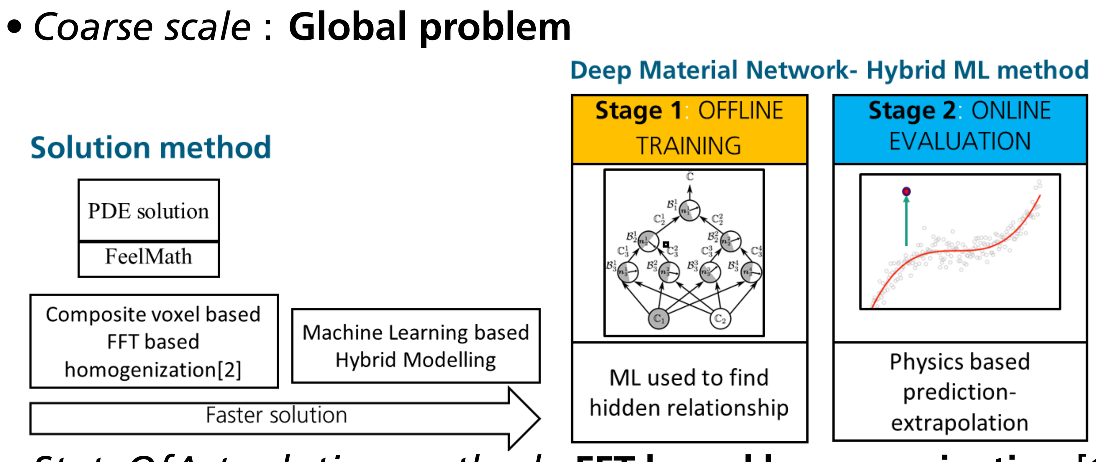
Deep Material Network (DMN)

Two scale approach



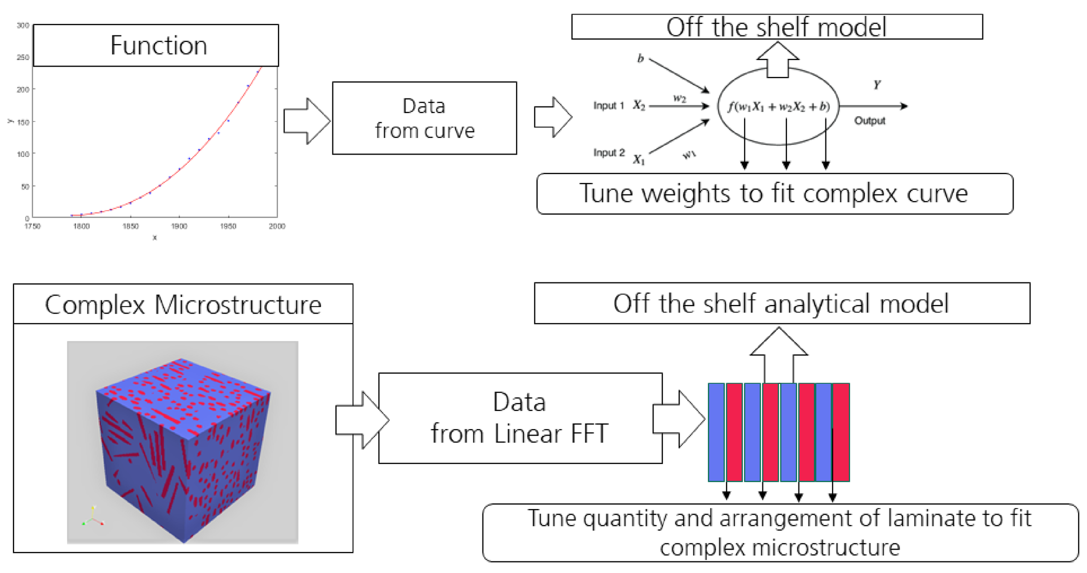
PDE cell problem
$0=\mathrm{div}_Y\sigma$, Y∈ μ-scale

- *Fine scale* : Cell problem ⇔ Homogenization of properties
- *Coarse scale* : Global problem



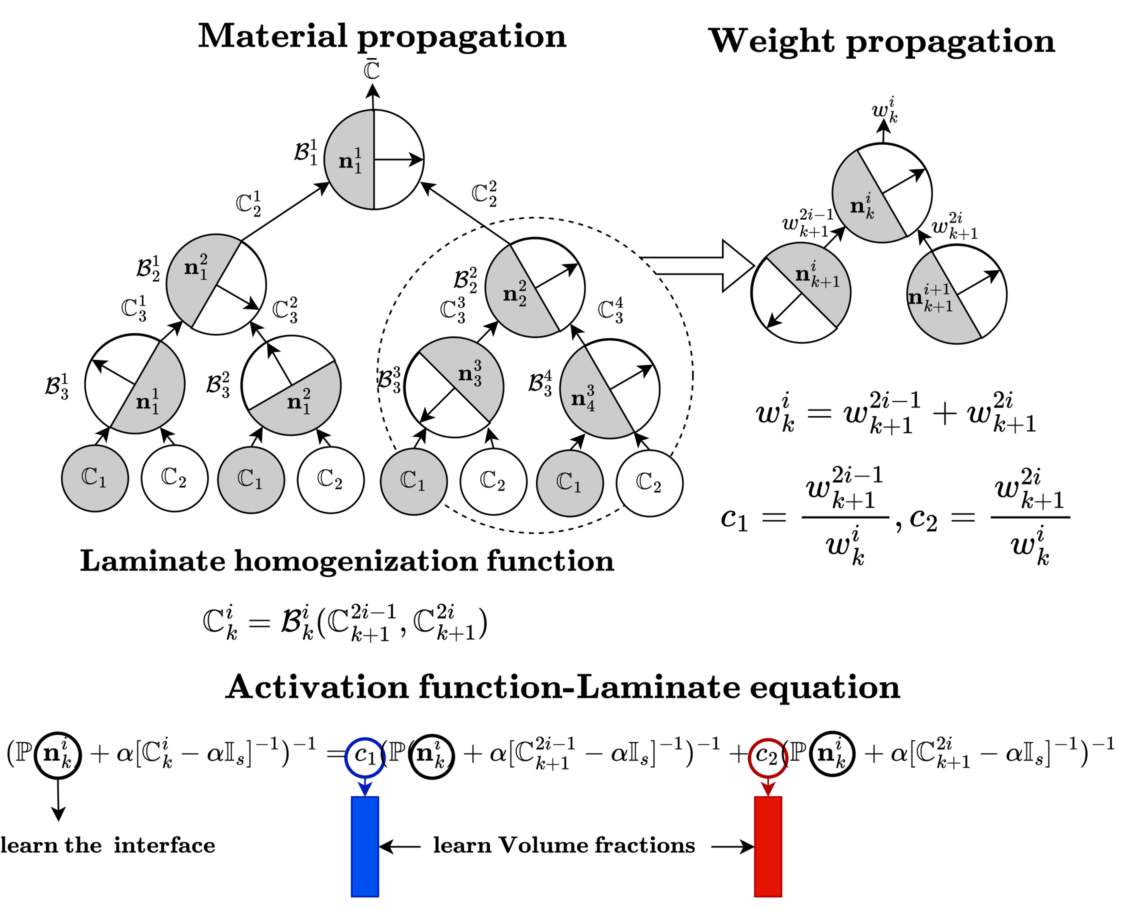
- *StateOfArt solution method* - FFT based homogenization [1]
- *Faster Data driven solution* - Deep Material Network [2].

Intuition of Linear elastic fitting



- Fit Topology like function [5]

Hierarchical laminate network



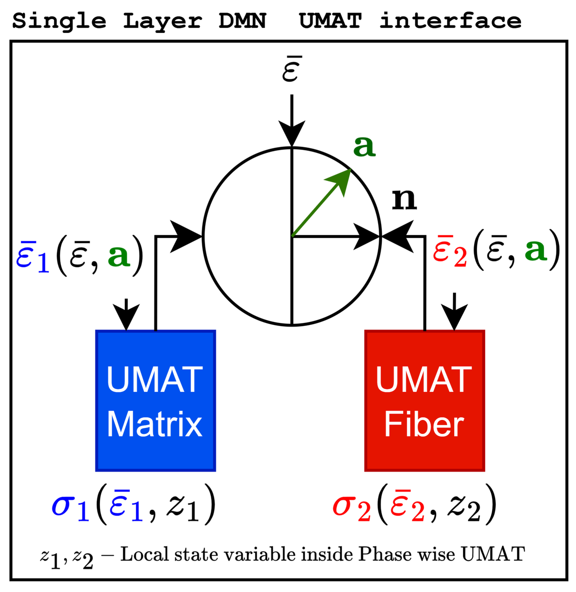
Problem: $J \to \min$
$J_{\mathbb{M}} = 0\ \forall \mathbb{M}$ – phase

$$J(\boldsymbol{n}, \boldsymbol{w}) = J_{Data} + \sum_{j=1}^{\mathbb{M}} \lambda_{\mathbb{M}} \cdot J_{\mathbb{M}}$$

$$J_{Data} = \frac{1}{N_b}\sum_{i=1}^{N_b}\left(\frac{\|\bar{\mathbb{C}}^i_{FFT} - \bar{\mathbb{C}}^i_{DMN}\|_1}{\|\bar{\mathbb{C}}^i_{FFT}\|_1}\right) \qquad J_{\mathbb{M}} = \left(\sum_{i=1}^{2^{k-1}} \frac{w_K^{i,\mathbb{M}}}{2^{k-1}} - c^{\mathbb{M}}\right)^2$$

- *Parameters*: w - Weights , **n** - Direction of laminate

Nonlinear extrapolation- DMN Online

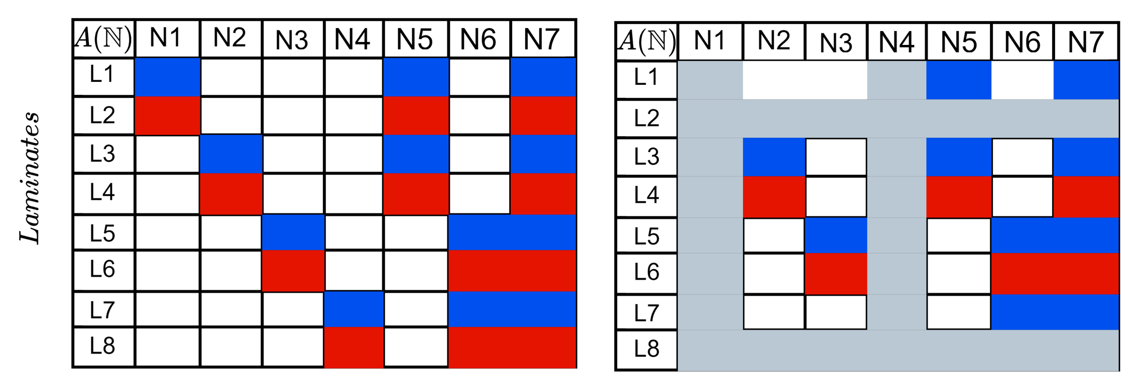


Kinematic decomposition
$\bar{\varepsilon}_1(\bar{\varepsilon}, \mathbf{a}) = \bar{\varepsilon} + c_2 \mathbb{N}\cdot\mathbf{a}$
$\bar{\varepsilon}_2(\bar{\varepsilon}, \mathbf{a}) = \bar{\varepsilon} - c_1 \mathbb{N}\cdot\mathbf{a}$
Interface momentum balance
$r(\mathbf{a}) = (\sigma_1 - \sigma_2) : \mathbb{N}$
Average stress
$\bar{\sigma} = c_1\sigma_1 + c_2\sigma_2$
Newton update scheme
$\Delta\mathbf{a} = -\frac{\partial r}{\partial \mathbf{a}}^{-1} \cdot r(\mathbf{a})$
a-Global state variable

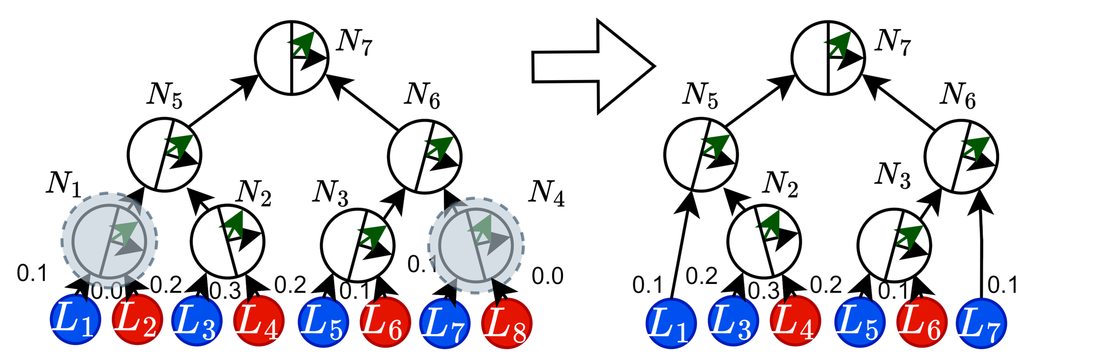
Vectorization and sparsification of Newton scheme

$$\frac{\partial r}{\partial a} = A^T \cdot W \cdot \frac{\partial \sigma}{\partial \varepsilon}_{local} \cdot A$$

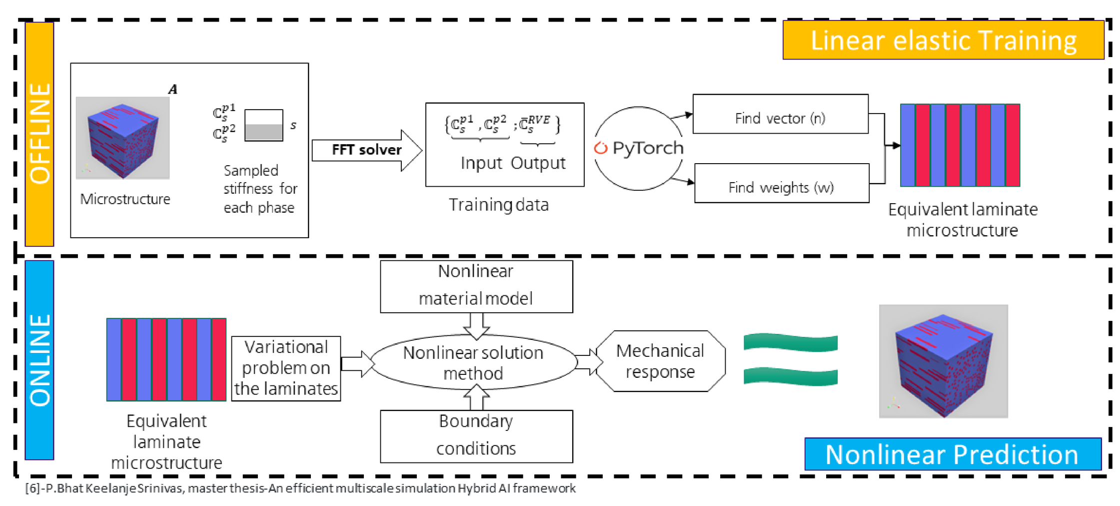
6 x 3 matrix block



Neuron elemination and pruning



Basic workflow and steps



Viscoelastic sampling and parameter choice

$$\mathbb{C}_f = 3\cdot K_f \cdot \mathbb{P}_1 + 2\cdot G_f \cdot \mathbb{P}_2$$

$$\mathbb{C}_M = 3\cdot K_0 \cdot \mathbb{P}_1 + 2\cdot\left(G_0 + \sum_{i=1}^{N_M} G_{M,i}\cdot(1-y_{s,i})^{\frac{\lambda}{\lambda_i}}\right)\cdot \mathbb{P}_2$$

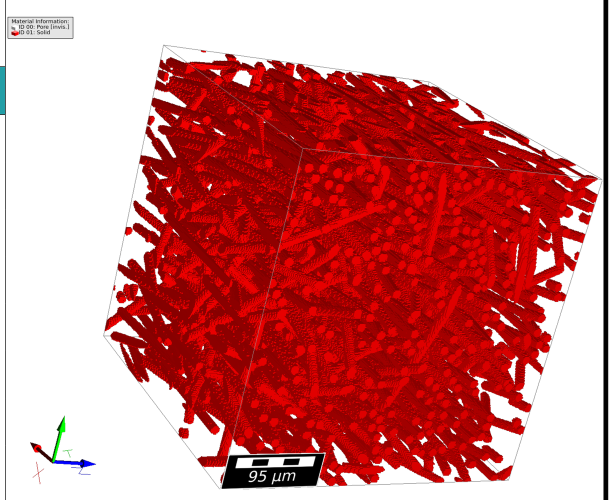
$$\mathbb{P}_1 = \mathbb{I}^{vol}, \mathbb{P}_2 = \mathbb{I}^{dev}, y_s \in U(0,1), N_M = 9$$

Parameters	Values
Microstructure	
Fiber length μm	200
Fiber diameter μm	10
Fiber volume fraction	16%
Number of voxels	256
Voxel length μm	1.5
Data	
Samples	1280
Train validation split	0.8
Test samples	51
Hyper-parameters	
N_b, batch size	8
$\lambda_{\mathbb{M}}$	100
Optimizer	Adam
Lr modulation	SGDR
$Epochs_{max}$	1000
Layer Depth	8
Lr α_{min}	0.0015
Lr α_{max}	0.015
Restart Epoch M	50

$$\eta(t) = \frac{\left\|\bar{\sigma}_t^{DMN} - \bar{\sigma}_t^{FFT}\right\|_1}{\left\|\bar{\sigma}_{t,max}^{FFT}\right\|_1}$$

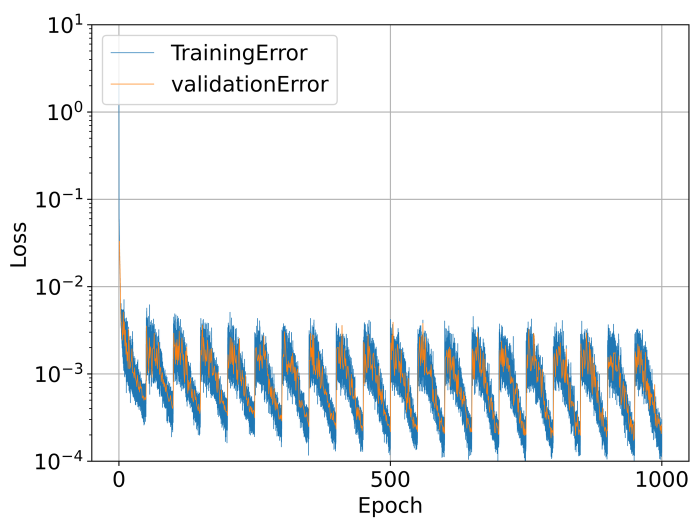
$$e = \frac{1}{N_b}\sum_{i=1}^{N_b}\left(\frac{\|\mathbb{C}_{act}^{hom} - \mathbb{C}_{pred}^{hom}\|_1}{\|\mathbb{C}_{act}^{hom}\|_1}\right)$$

Figure 1: (0.8,0.1)



Nonlinear Tests chosen	
Uniaxial testing	ε_{max} = 4%
$\dot{\varepsilon}$ = 0.0005	6 directions
$\dot{\varepsilon}$ = 0.005	6 directions
$\dot{\varepsilon}$ = 0.05	6 directions
$\dot{\varepsilon}$ = 0.5	6 directions
Creep testing	20 seconds
ε=4%	6 directions
Total tests	30

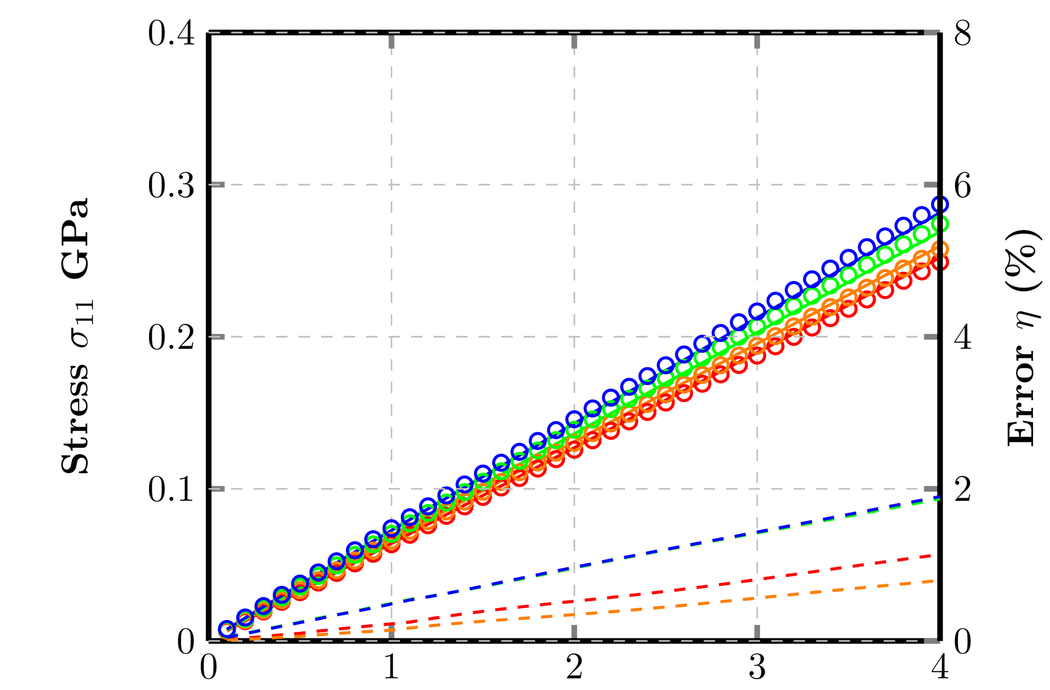
Offline hyper-parameter-tuning



Time	& Jobs
data	11.25 hours
threads	48
Jobs	5 batch
Training	1.5 hours
threads	1

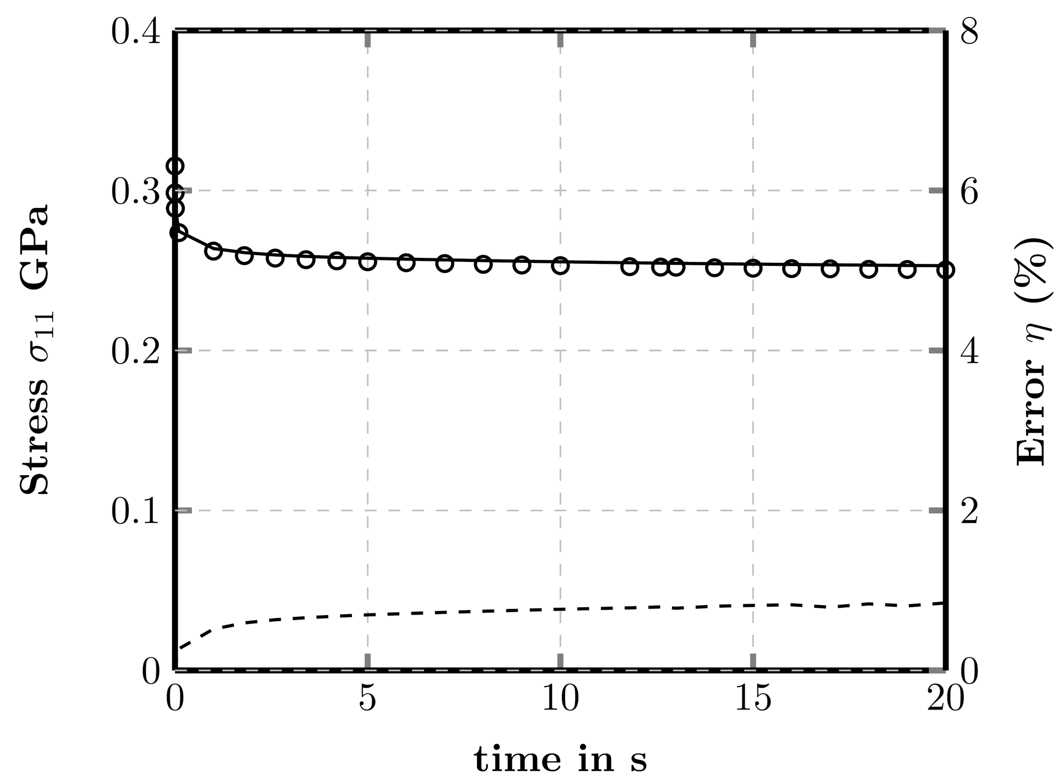
Results and Takeaways

- Inelastic error, $\eta(t) < 2\%$.
- DMN speed $<$100 sec with 1 thread.
- Full field FFT~ 51 hours with 24 threads.
- For viscoelasticity, total speed-up factor of 44064.
- Achieved 8 layered DMN with state-of-the-art speeds and accuracies.



Uniaxial extension in principal fiber direction

DMN∘FFT   Error η (%)



Relaxation test in principal fiber direction

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References

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