

# Learning Constitutive Models in Multiscale Modeling of Materials

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# Outline

- Problem Statement
- Methodology
- Numerical Examples
- Conclusion & Outlook

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# Problem Statement

Macroscopic Problem: Find  $\bar{\mathbf{u}}(\bar{\mathbf{X}})$

$$\text{Div } \bar{\mathbf{P}}(\bar{\mathbf{u}}) = \mathbf{0} \quad \text{on } \bar{\Omega},$$

$$\bar{\mathbf{P}} \bar{\mathbf{N}} = \bar{\mathbf{t}}_0 \quad \text{on } \partial \bar{\Omega}^N,$$

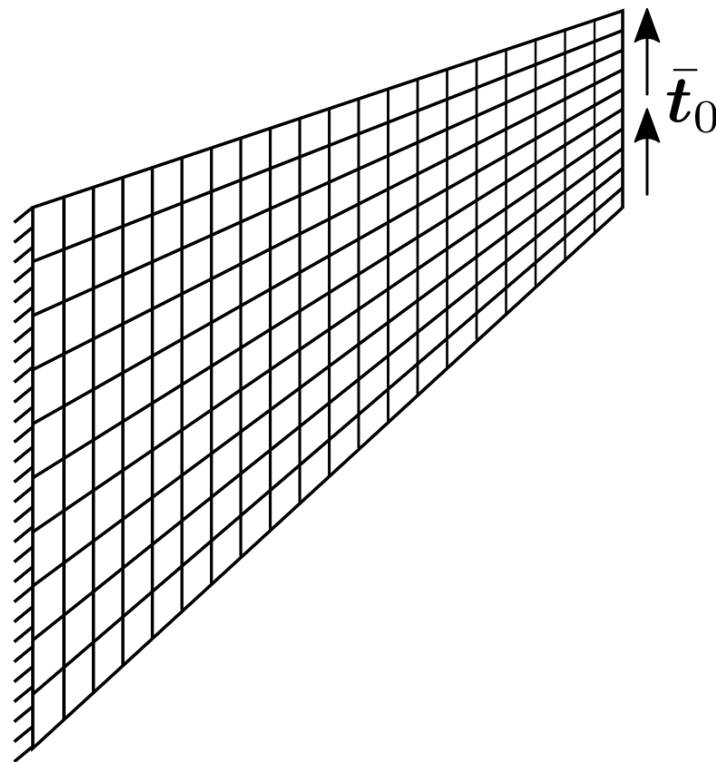
$$\bar{\mathbf{u}} = \bar{\mathbf{u}}_0 \quad \text{on } \partial \bar{\Omega}^D,$$

Constitutive Model

$$\bar{\mathbf{P}} = \bar{\mathbf{P}}(\bar{\mathbf{F}}, \mu)$$

$$\bar{\mathbf{F}} = \mathbf{I} + \frac{\partial \bar{\mathbf{u}}}{\partial \bar{\mathbf{X}}}$$

$$\bar{\mathbf{A}} = \frac{\partial \bar{\mathbf{P}}(\bar{\mathbf{F}}, \mu)}{\partial \bar{\mathbf{F}}}$$



[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

# Problem Statement

Microscopic Problem: Find  $u(\mathbf{X})$

$$\text{Div} \mathbf{P}(\mathbf{u}) = \mathbf{0} \quad \text{on } \Omega$$

$$\mathbf{u} = \underbrace{(\bar{\mathbf{F}} - \mathbf{I})\mathbf{X}}_{\text{mean}} + \underbrace{\mathbf{w}(\mathbf{X})}_{\text{fluctuation}}$$

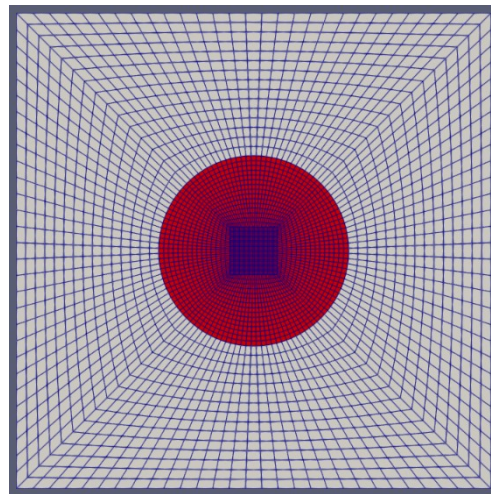
Neo-Hookean material

$$W(\mathbf{F}, \mu) = C_1 (\text{Tr}(\mathbf{F}^T \mathbf{F}) - 3 - 2 \ln(\det \mathbf{F})) + D_1 (\det \mathbf{F} - 1)^2$$

$$\mathbf{P}(\mathbf{F}, \mu) = \frac{\partial W}{\partial \mathbf{F}}$$

$$\mathbf{A}(\mathbf{F}, \mu) = \frac{\partial \mathbf{P}}{\partial \mathbf{F}}$$

$\bar{\mathbf{F}}$  loading: macroscopic deformation gradient  
 $\mu$  parameters: material & geometry



[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

# Problem Statement

Scale Coupling

$$\langle \bullet \rangle = |\Omega|^{-1} \int_{\Omega} \bullet \, dV$$

Hill-Mandel Condition

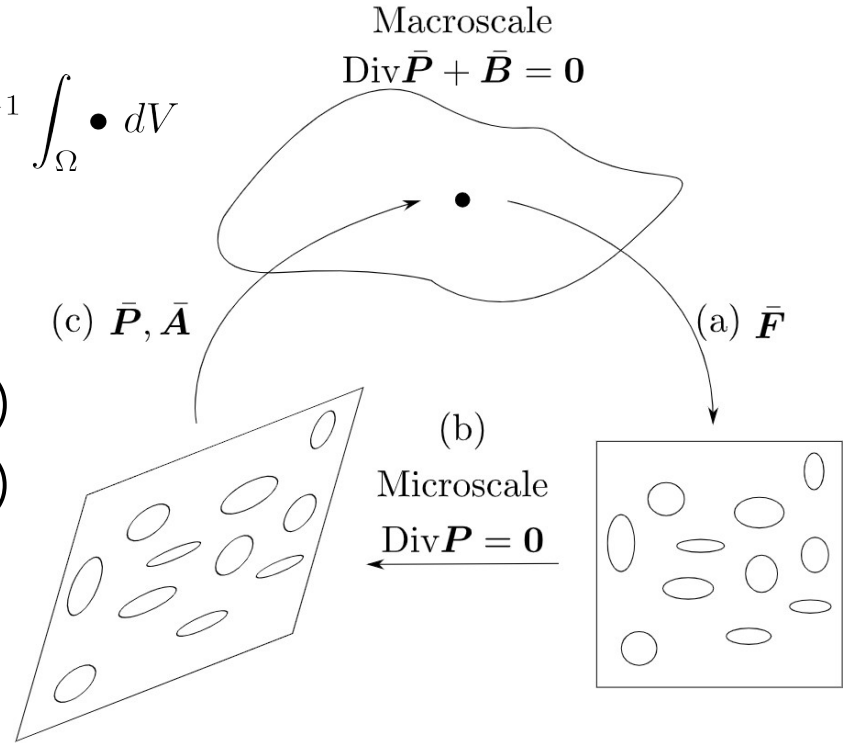
$$\langle \mathbf{P} : \delta \mathbf{F} \rangle = \bar{\mathbf{P}} : \delta \bar{\mathbf{F}}$$

$$\Rightarrow \begin{array}{lll} w = 0 & \text{on } \partial\Omega & \text{(KBC)} \\ w \text{ periodic} & \text{on } \partial\Omega & \text{(PBC)} \end{array}$$

Effective Quantities

$$\bar{\mathbf{P}} = \langle \mathbf{P} \rangle$$

$$\bar{\mathbf{A}} \neq \langle \mathbf{A} \rangle$$



[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

# Problem Statement

- Full two-scale simulations → **too expensive**  
(multi-query contexts: optimization, materials design, etc.)
- **Non-intrusive and accurate approximation of the microscopic stress field for different parameters**
- Obtain rapidly **effective stress** → reducing to a **single-scale** problem

$$P(X, \bar{F}, \mu), \quad \bar{P}(\bar{F}, \mu)$$

- **Accurate effective stiffness and sensitivities**

$$\bar{A} = \frac{\partial \bar{P}(\bar{F}, \mu)}{\partial \bar{F}}, \quad \frac{\partial \bar{P}(\bar{F}, \mu)}{\partial \mu}$$

# Methodology

## Intrusive RB Method

### Approximate displacement field

$$u(\mathbf{X}, \bar{\mathbf{F}}, \mu) \approx \sum_{l=1}^L \alpha_l(\bar{\mathbf{F}}, \mu) \Phi_l(\mathbf{X}) = \Phi \alpha \text{ with } \Phi(\mathbf{X}) \text{ RB basis functions}$$

### Reduced problem

$$\mathbf{f}(\Phi \alpha) = 0$$

Need hyperreduction!

$$\Phi^T \boxed{Df|_{\Phi \alpha^k}} \Phi \Delta \alpha = -\Phi^T \boxed{f(\Phi \alpha^k)}$$
$$\alpha^{k+1} = \alpha^k + \Delta \alpha$$

- **Hyperreduction**  
(convergence problems)
- **Intrusive**  
(requires access to the microscopic solver)

[Yvonnet, J. and He, Q.C., 2007, JCP 223]

[Radermacher, A., et al., 2016, AMSES 3(1)]

[Hernández, J. A., et al., 2014, CMAME 276]

[Soldner, Dominic, et al., 2017, Comput. Mech. 60(4)]

# Methodology

## Non-Intrusive RB Method

[Guo, M. and Hesthaven, J.S., 2018, CMAME 341]

[Kast, M., Guo, M. and Hesthaven, J.S., 2020, CMAME 364]

[Swischuk, Renee, et al., 2019, Comput Fluids 179]

### Approximate displacement field

$$u(\mathbf{X}, \bar{\mathbf{F}}, \mu) \approx \sum_{l=1}^L \alpha_l(\bar{\mathbf{F}}, \mu) \Phi_l(\mathbf{X}) = \Phi \alpha \text{ with } \Phi(\mathbf{X}) \text{ RB basis functions}$$

Instead of solving reduced system, perform a regression to obtain

For a new pair  $(\bar{\mathbf{F}}, \mu)$ , the coefficients  $\alpha$  can be directly obtained

$$\hat{\alpha}_l : \mathcal{P} \rightarrow \mathbb{R} : (\bar{\mathbf{F}}, \mu) \mapsto \hat{\alpha}_l(\bar{\mathbf{F}}, \mu)$$



# Methodology

## Non-Intrusive RB Method

[Guo, M. and Hesthaven, J.S., 2018, CMAME 341]

[Kast, M., Guo, M. and Hesthaven, J.S., 2020, CMAME 364]

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### Approximate displacement field

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To obtain stresses, gradient of  $u$  is needed, and evaluation of the constitutive model

- **Intrusive:** Need to implement material model
- **Slow:** Need to evaluate material model  $N_{qp}$  times

Idea: Approximate stress field directly!

$$P(\mathbf{X}, \bar{\mathbf{F}}, \mu) \approx \sum_{l=1}^L \alpha_l(\bar{\mathbf{F}}, \mu) B_l(\mathbf{X})$$

# Methodology

## Proper Orthogonal Decomposition (POD)

1. Collect stress snapshots
2. Compute correlation matrix

$$\mathbf{S} = [\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \dots, \mathbf{P}^{(N_{\text{pod}})}]$$

$$C_{ij} = \left( \mathbf{P}^{(i)}, \mathbf{P}^{(j)} \right)_{L^2(\Omega)} = \int_{\Omega} \mathbf{P}^{(i)} : \mathbf{P}^{(j)} dV$$

3. Compute the eigenvalues  $\lambda_l$  and eigenvectors  $\mathbf{v}_l$  of  $\mathbf{C}$
4. Compute the basis functions

$$\mathbf{B}_l = \frac{1}{\sqrt{\lambda_l}} \mathbf{S} \mathbf{v}_l \quad (\mathbf{B}_i, \mathbf{B}_j)_{L^2(\Omega)} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$$\Rightarrow \mathbf{P}^{\text{RB}}(\mathbf{X}, \bar{\mathbf{F}}, \mu) = \sum_{l=1}^L \alpha_l(\bar{\mathbf{F}}, \mu) \mathbf{B}_l(\mathbf{X})$$

[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

# Methodology

## Effective Quantities

$\int_{\Omega} B_l(\mathbf{X}) dV$  can be computed offline!

$$\bar{\mathbf{P}} = \langle \mathbf{P}^{\text{RB}} \rangle = |\Omega|^{-1} \int_{\Omega} \mathbf{P}^{\text{RB}} dV = |\Omega|^{-1} \sum_{l=1}^L \alpha_l(\bar{\mathbf{F}}, \mu) \int_{\Omega} B_l(\mathbf{X}) dV$$

$$\bar{\mathbf{A}} = \frac{\partial \bar{\mathbf{P}}}{\partial \bar{\mathbf{F}}} = |\Omega|^{-1} \sum_{l=1}^L \int_{\Omega} B_l(\mathbf{X}) dV \otimes \frac{\partial \alpha_l(\bar{\mathbf{F}}, \mu)}{\partial \bar{\mathbf{F}}}$$

## Sensitivities

$$\frac{\partial \bar{\mathbf{P}}}{\partial \mu} = |\Omega|^{-1} \sum_{l=1}^L \int_{\Omega} B_l(\mathbf{X}) dV \otimes \frac{\partial \alpha_l(\bar{\mathbf{F}}, \mu)}{\partial \mu}$$

$\Rightarrow$  Construct  $\hat{\alpha}_l(\bar{\mathbf{F}}, \mu), \frac{\partial \hat{\alpha}_l(\bar{\mathbf{F}}, \mu)}{\partial \bar{\mathbf{F}}}, \frac{\partial \hat{\alpha}_l(\bar{\mathbf{F}}, \mu)}{\partial \mu}$  with Gaussian Process Regression!

# Methodology

[Guo, M. and Hesthaven, J.S., 2018, CMAME 341]

[Rasmussen, C.E., 2003, *Summer school on machine learning*]

## Gaussian Process Regression (GPR)

Given some data  $\{\mathbf{X}^{(i)}, y^{(i)}\}_{i=1}^N$ , we want to find a scalar regression function which is distributed as a Gaussian Process with zero mean function and kernel  $k_{\theta}(\mathbf{X}, \mathbf{X}')$

$$f \sim \mathcal{GP}(0, k_{\theta}(\mathbf{X}, \mathbf{X}'))$$

Automatic relevance determination (ARD) squared exponential kernel

$$k_{\theta}(\mathbf{X}, \mathbf{X}') = \sigma_f^2 \exp \left( -\frac{1}{2} \sum_{k=1}^d \frac{(X_k - X'_k)^2}{l_k^2} \right)$$

# Methodology

[Guo, M. and Hesthaven, J.S., 2018, CMAME 341]

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## Gaussian Process Regression (GPR)

Given some data  $\{\mathbf{X}^{(i)}, y^{(i)}\}_{i=1}^N$ , we want to find a scalar regression function which is distributed as a Gaussian Process with zero mean function and kernel  $k_{\theta}(\mathbf{X}, \mathbf{X}')$

$$f^* | (\mathbf{X}, \mathbf{y}) \sim \mathcal{GP}(m^*, k^*),$$

$$m^*(\mathbf{x}) = \mathbf{k}_{\theta}(\mathbf{X}, \mathbf{x})^T \mathbf{k}_{\theta}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{y}(\mathbf{X}),$$

$$k^*(\mathbf{x}, \mathbf{x}') = k_{\theta}(\mathbf{x}, \mathbf{x}') - \mathbf{k}_{\theta}(\mathbf{X}, \mathbf{x})^T \mathbf{k}_{\theta}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{k}_{\theta}(\mathbf{X}, \mathbf{x}')$$

$$\text{where } \mathbf{k}_{\theta}(\mathbf{X}, \mathbf{x}) = [k_{\theta}(\mathbf{X}^{(1)}, \mathbf{x}), k_{\theta}(\mathbf{X}^{(2)}, \mathbf{x}), \dots, k_{\theta}(\mathbf{X}^{(N)}, \mathbf{x})]^T$$

$$\mathbf{k}_{\theta}(\mathbf{X}, \mathbf{X}) = [k_{\theta}(\mathbf{X}^{(i)}, \mathbf{X}^{(j)})]_{i,j=1}^N$$

$$\mathbf{y}(\mathbf{X}) = [f(\mathbf{X}^{(1)}), f(\mathbf{X}^{(2)}), \dots, f(\mathbf{X}^{(N)})]^T$$

# Numerical Examples

[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

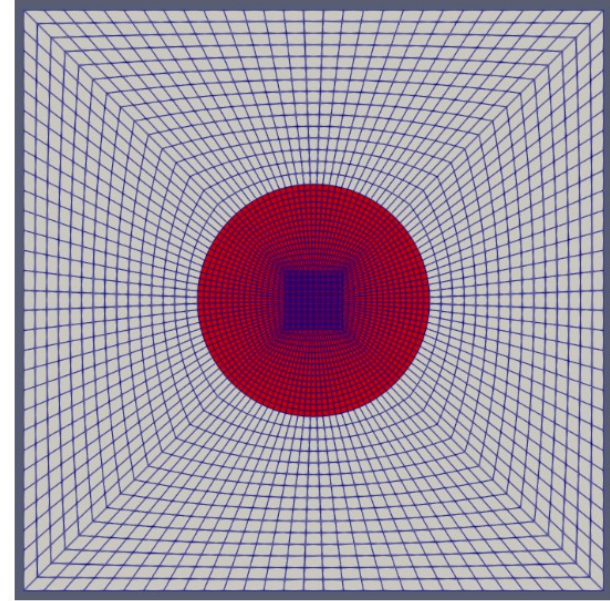
## Fiber reinforced microstructure

- 4321 eight-node elements with 4 quadrature points
- Volume fraction of fiber is 12.56%
- Matrix material  $C_1^{\text{mat}} = D_1^{\text{mat}} = 1$
- Fiber material  $C_1^{\text{fib}} = D_1^{\text{fib}} \in [50, 150]$
- Deformations  $\bar{\mathbf{U}} - \mathbf{I} \in [-0.3, 0.3]$
- 500 training snapshots (Sobol sequence)
- 1000 testing snapshots (uniformly random)
- P-PODGPR Error

$$\epsilon_{\bar{\mathbf{P}}} := \frac{\|\bar{\mathbf{P}}^{\text{HF}} - \hat{\bar{\mathbf{P}}}^{\text{RB}}\|_{\text{F}}}{\|\bar{\mathbf{P}}^{\text{HF}}\|_{\text{F}}}$$

- Projection Error

$$\epsilon_{\bar{\mathbf{P}}} := \frac{\|\bar{\mathbf{P}}^{\text{HF}} - \bar{\mathbf{P}}^{\text{RB}}\|_{\text{F}}}{\|\bar{\mathbf{P}}^{\text{HF}}\|_{\text{F}}}$$



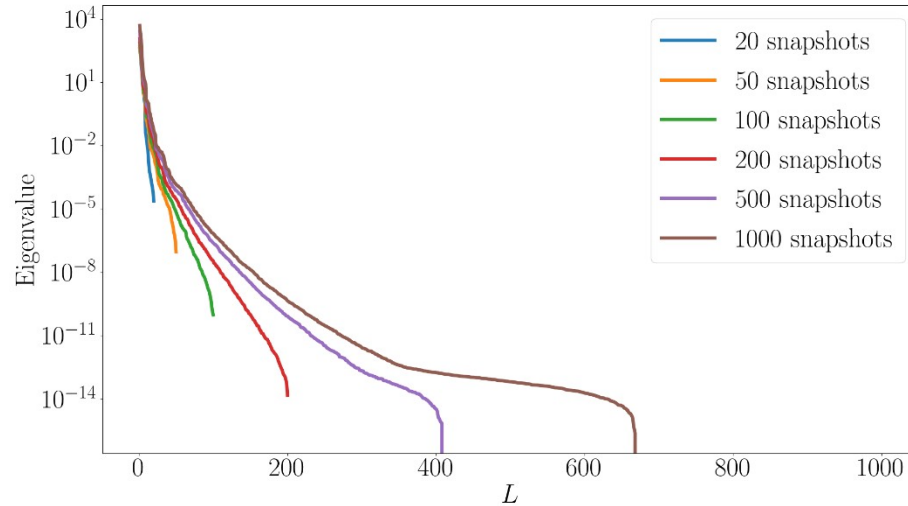
$$W(\mathbf{F}, \boldsymbol{\mu}) = C_1(\text{Tr}(\mathbf{F}^T \mathbf{F}) - 3 - 2 \ln(\det \mathbf{F})) + D_1(\det \mathbf{F} - 1)^2$$

# Numerical Examples

[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Fiber reinforced microstructure

POD for different numbers of training snapshots



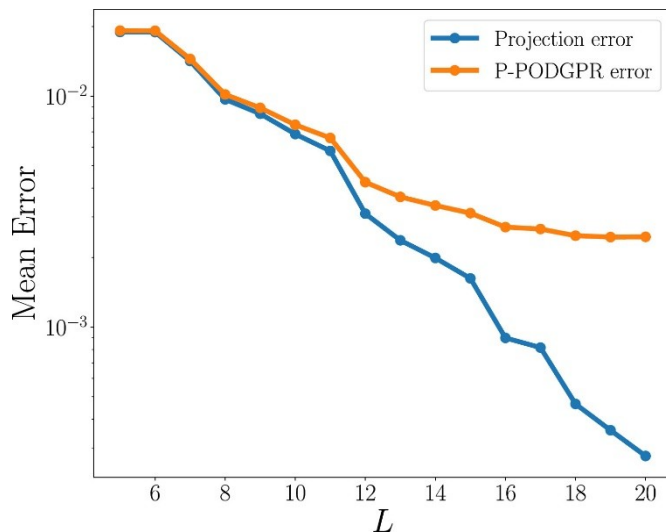
With  $L = 20$ , 
$$\frac{\sum_{i=1}^L \lambda_i}{\sum_{i=1}^N \lambda_i} = 0.9999$$

# Numerical Examples

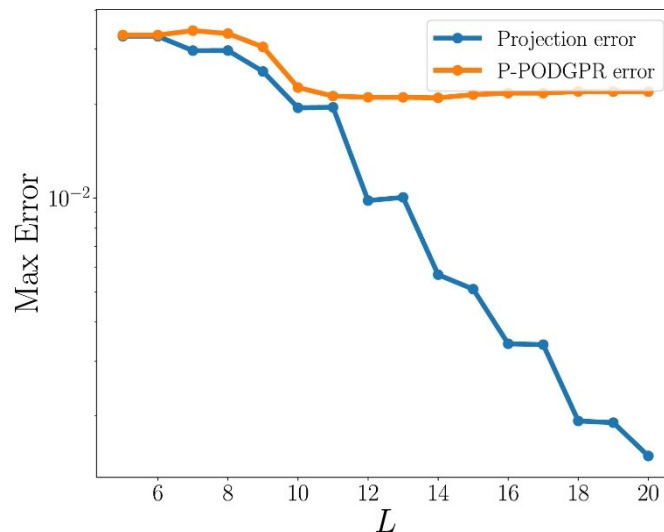
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Fiber reinforced microstructure

Test error in effective stress for 200 training snapshots



Mean error  $\approx 0.003$



Max error  $\approx 0.011$

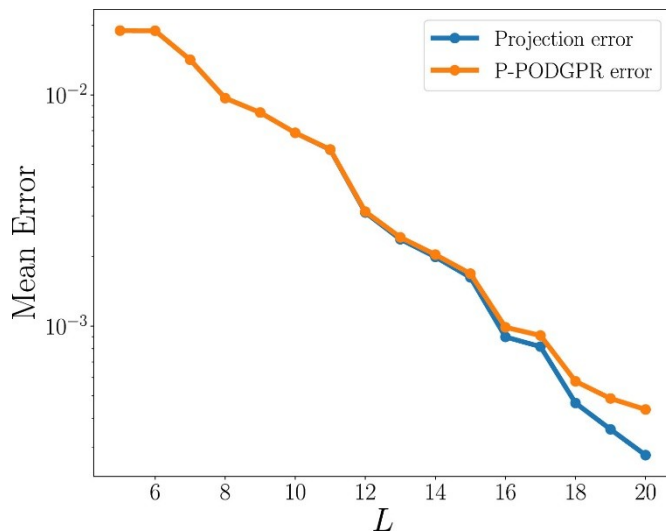


# Numerical Examples

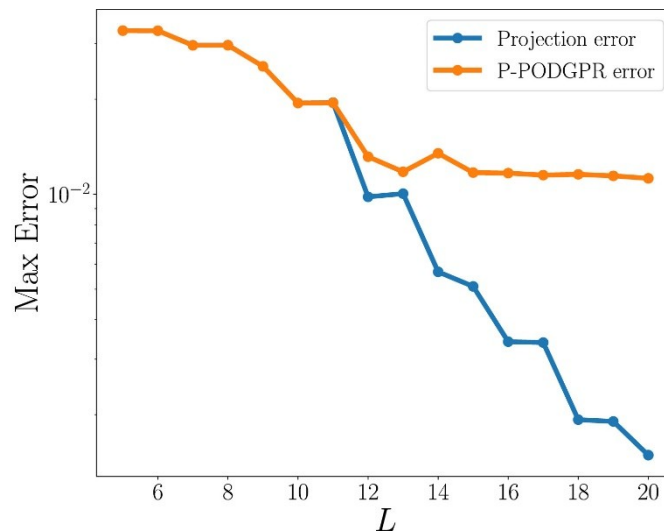
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Fiber reinforced microstructure

Test error in effective stress for 500 training snapshots



Mean error  $\approx 0.0004$



Max error  $\approx 0.01$

# Numerical Examples

[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Fiber reinforced microstructure

- Comparison with a neural network (Multilayer Perceptron) that is trained with pairs of  $\{\bar{U}^{(i)}, \bar{P}^{(i)}\}_{i=1}^N$  with  $N = 500$  training snapshots
- Trained with Adam optimizer with learning rate of  $10^{-4}$ , batch size of 32 and Mean Squared Error Loss function for different architectures
- ELU activation function was applied after every layer apart from last layer

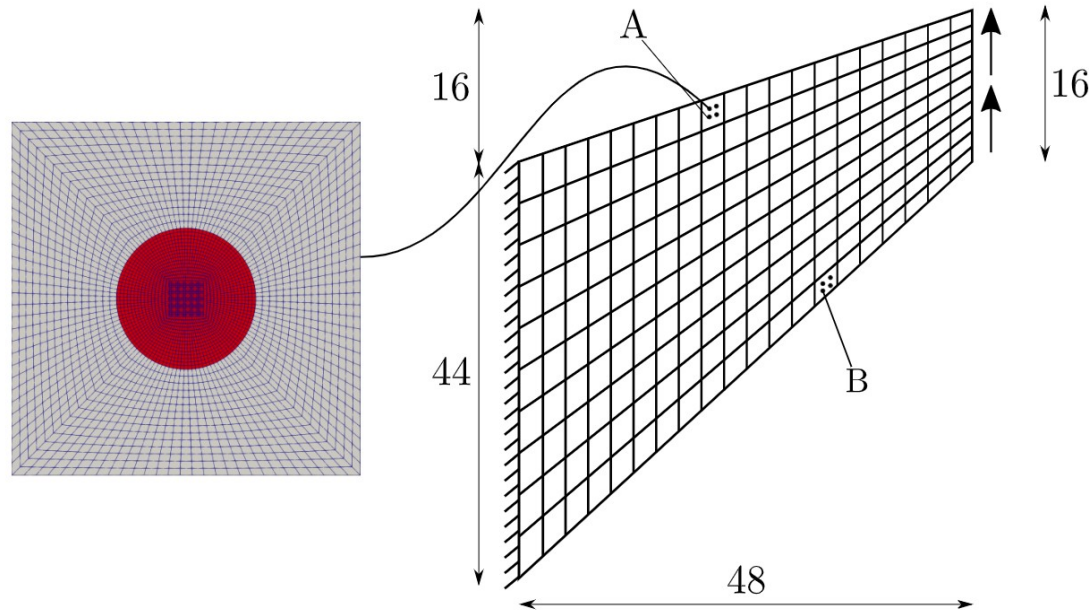
Architecture	Validation Loss	$\epsilon_{\bar{P}}^{\text{mean}}$	$\epsilon_{\bar{P}}^{\text{max}}$
$N_h = 1, N_n = 20$	$1.7 \times 10^{-6}$	0.0077	0.0368
$N_h = 1, N_n = 50$	$8.55 \times 10^{-7}$	0.0056	0.0289
$N_h = 2, N_n = 20$	$5.36 \times 10^{-7}$	0.0047	<b>0.0176</b>
$N_h = 2, N_n = 50$	<b><math>2.97 \times 10^{-7}</math></b>	<b>0.0039</b>	0.0206
$N_h = 2, N_n = 100$	$7.91 \times 10^{-7}$	0.0052	0.0315

⇒ P-PODGPR outperforms all neural networks, while also being able to recover the microscopic stress field

# Numerical Examples

[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem



# Numerical Examples

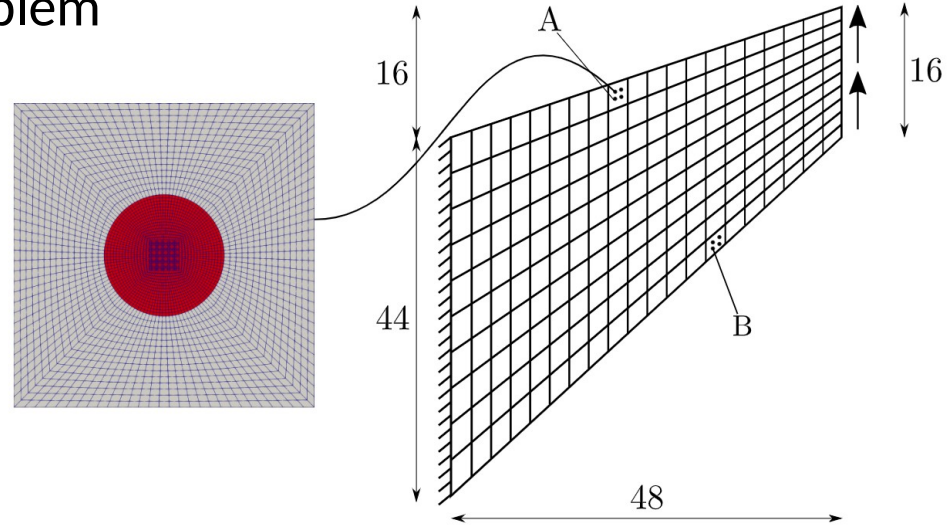
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

- 200 four-node elements with 4 quadrature points
- Vertical traction of 0.1 on right edge
- Left edge is fixed
- Matrix material  $C_1^{\text{mat}} = D_1^{\text{mat}} = 1$
- Fiber material  $C_1^{\text{fib}} = D_1^{\text{fib}} = 100$
- Surrogate model trained with 200 snapshots
- Relative error to compare microscopic stresses

$$\epsilon_{P_{yx}} := |P_{yx}^{\text{FE2}} - P_{yx}^{\text{ROM}}| / \langle |P_{yx}^{\text{FE2}}| \rangle$$

$\langle |P_{yx}^{\text{FE2}}| \rangle$ : Averaged absolute stress



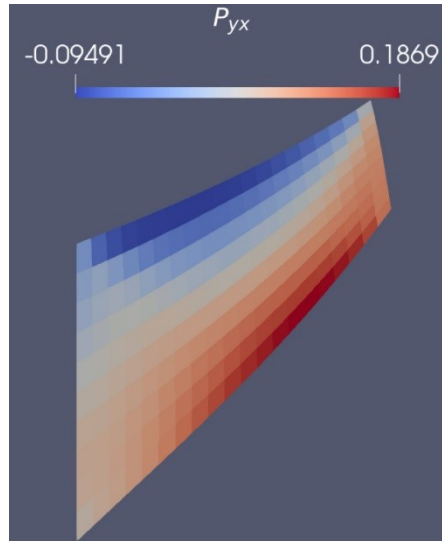
$$W(\mathbf{F}, \mu) = C_1(\text{Tr}(\mathbf{F}^T \mathbf{F}) - 3 - 2 \ln(\det \mathbf{F})) + D_1(\det \mathbf{F} - 1)^2$$

# Numerical Examples

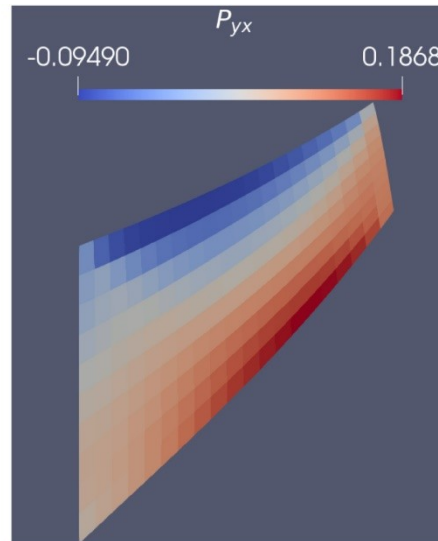
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

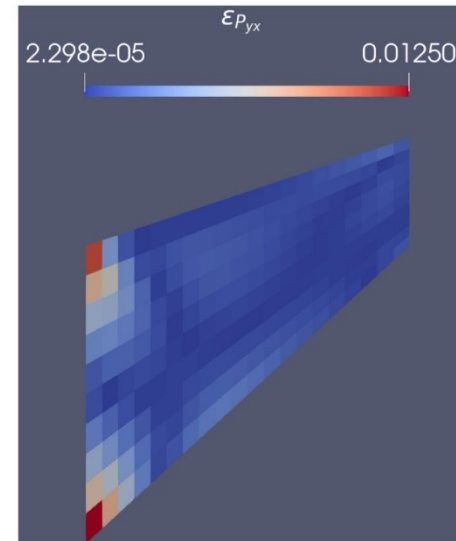
Macroscopic stress component  $P_{yx}$



(a)  $FE^2$



(b) FE with P-PODGPR



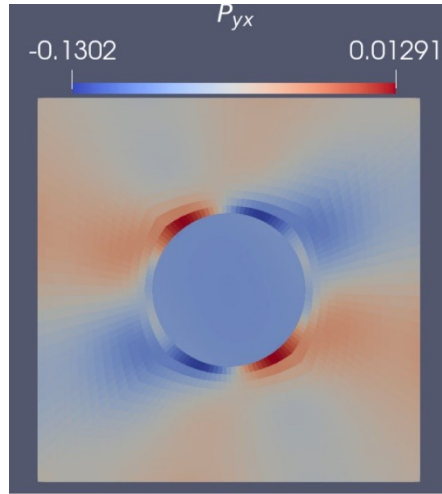
(c) Relative error

# Numerical Examples

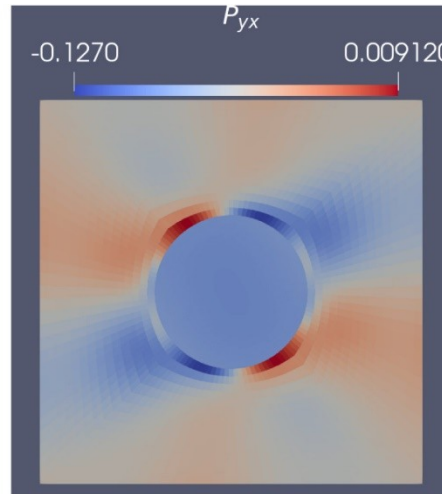
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

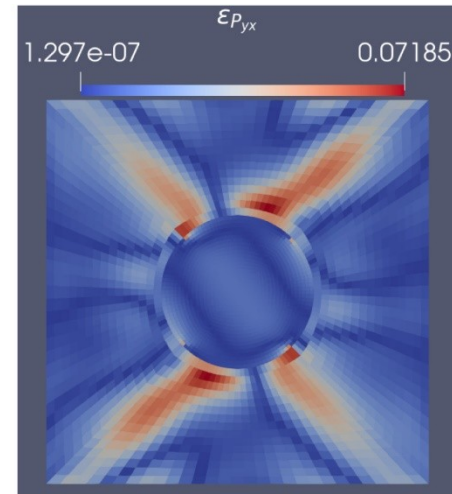
Microscopic stress component  $P_{yx}$  at point A



(a)  $FE^2$



(b) FE with P-PODGPR



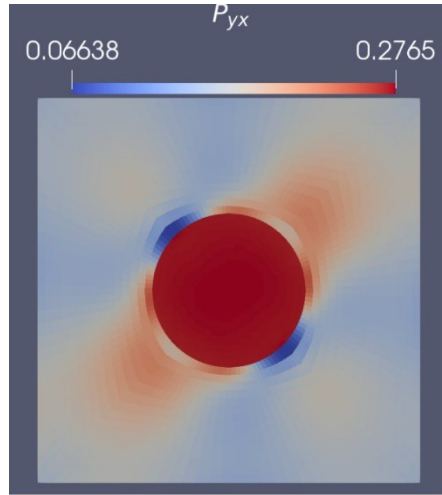
(c) Relative error

# Numerical Examples

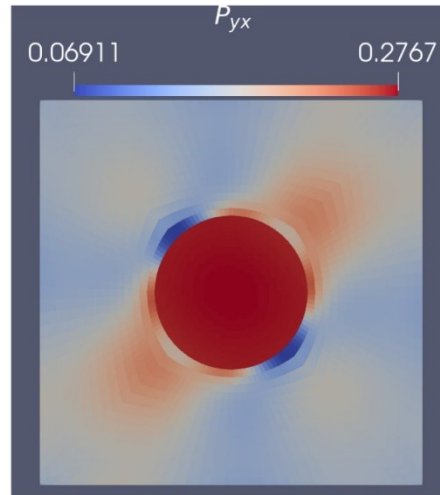
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

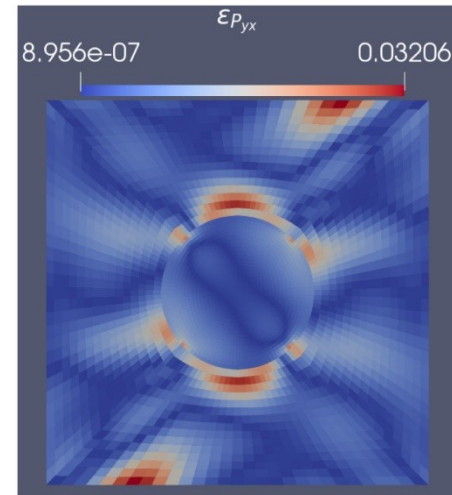
Microscopic stress component  $P_{yx}$  at point B



(a)  $FE^2$



(b) FE with P-PODGPR



(c) Relative error

# Numerical Examples

[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

	FE <sup>2</sup>	FE with P-PODGPR
Snapshot generation	-	60 min
POD + GPR	-	1 min
Online simulation	4800 min	1 min

⇒ Online speedup of the order of 1000



# Conclusion & Outlook

## Summary

- Novel method based on non-intrusive reduced basis method
- Validated on 2D composite microstructure and multiscale application
- High accuracy and online speedup
- Sensitivities are available and can be used for optimization

## Outlook

- Geometrical parameters
- Dissipative constitutive models (Plasticity, Damage)
- Test on 3D problems

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# References

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