

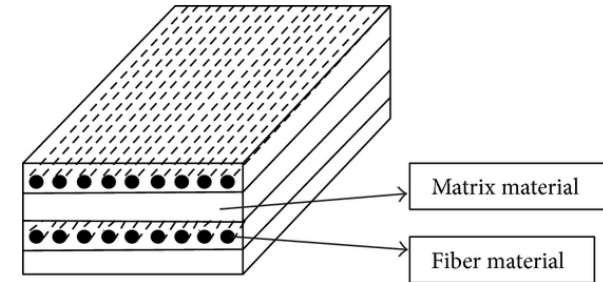
# A reduced basis method for accelerating parameterized non-linear microstructures

M2I MEETING MATERIALS 2022 05.04.2022

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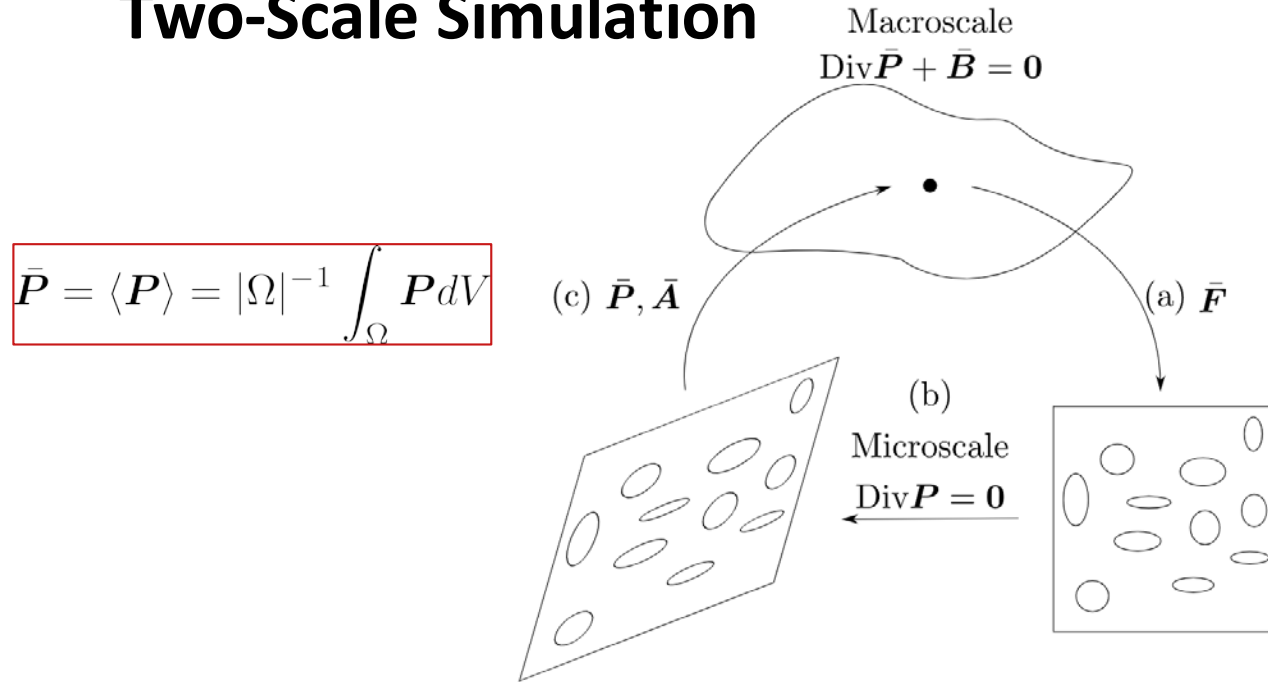
# Motivation

- Understanding structure-property relations
  - What is the influence of the microstructure onto macroscopic behavior?
  - What is the optimal microstructure for a given application?
- Applications
  - **Design:** Composite Materials, Metamaterials
  - **Reliability Analysis:** Effect of microscopic variations
  - **Design of Production Processes:** Effect of external factors



([https://www.researchgate.net/figure/Composite-material-with-fiber-and-matrix\\_fig13\\_258393869](https://www.researchgate.net/figure/Composite-material-with-fiber-and-matrix_fig13_258393869))

# Two-Scale Simulation



Full two-scale simulation → **too expensive** (multi-query contexts such as optimization, material design, etc.)

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

# Microscopic Problem

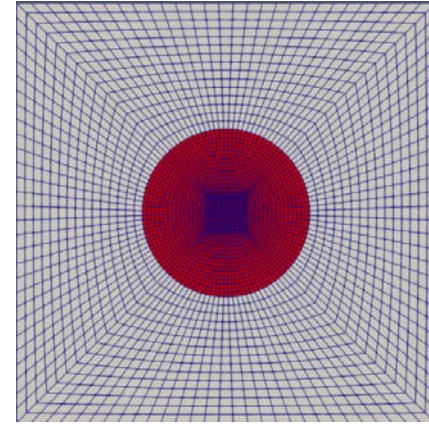
$$\text{Div} \mathbf{P}(\mathbf{u}) = \mathbf{0} \quad \text{on } \Omega$$

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

$\mathbf{w}$  periodic on  $\partial\Omega$

Several problem parameters:

- **3 loading parameters**
- Each phase has **2 material parameters**
- Each phase can **be geometrically parameterized**
- (Interfaces between phases could be modelled)



Each phase modelled as hyperelastic material

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

$$\mathbf{P}(\mathbf{F}, \lambda) = \frac{\partial W}{\partial \mathbf{F}} \quad \lambda = [C_1, D_1]^T$$

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

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

# Methodology

## Related Works

- Fast Fourier Transform
  - [Moulinec, H., Suquet, P., 1997, CMAME]
- (Nonuniform) Transformation Field Analysis
  - [Michel, J., Suquet, P., 2003, Int J Solids Struct]
  - [Fritzen, F., Leuschner, M., 2013, CMAME]
- Reduced Basis Method
  - [Hernández, J.A., et al., 2014, CMAME]
  - [Radermacher, A., Reese, S., 2016, Int J Nume Meth Eng]
  - [Yvonnet, J., He, Q., 2007, JCP]

Only considered loading parameters:

- Can speed up one forward simulation
- Cannot be used for optimization

# Methodology

- Learn effective constitutive model from precomputed microscopic simulations

→ reduce to two **single-scale** problems

(Offline Stage)

- Learn regression model for **effective stress and effective stiffness**

$$\bar{P}(\bar{\mathbf{U}}, \lambda, \mu), \quad \bar{\mathbf{A}} = \frac{\partial \bar{P}(\bar{\mathbf{U}}, \lambda, \mu)}{\partial \bar{\mathbf{U}}}$$

$\bar{\mathbf{U}}$  : Loading parameters

$\lambda$  : Material parameters

$\mu$  : Geometrical parameters

- **Effective sensitivities**

$$\frac{\partial \bar{P}(\bar{\mathbf{U}}, \lambda, \mu)}{\partial \lambda}, \quad \frac{\partial \bar{P}(\bar{\mathbf{U}}, \lambda, \mu)}{\partial \mu}$$

[Wu, L., et al., 2020, CMAME 369]

[Mozaffar, M., et al., 2019, PNAS 116]

# Methodology

- Many samples need to be generated
- Microscopic quantities cannot be recovered
- Physics might not be fulfilled
- Instead: Approximation of the microscopic **stress field**

$$P(X; \bar{U}, \lambda, \mu)$$

$\bar{U}$  : Loading parameters

$\lambda$  : Material parameters

$\mu$  : Geometrical parameters

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

$$\frac{\partial \bar{P}(\bar{U}, \lambda, \mu)}{\partial \lambda}, \quad \frac{\partial \bar{P}(\bar{U}, \lambda, \mu)}{\partial \mu}$$

# Methodology

## Idea: Reduced Basis Method

- Approximate the microscopic stress field with a linear combination of global basis functions with parameter-dependent coefficients

$$\mathbf{P} \approx \mathbf{P}^{\text{RB}}(\mathbf{X}; \bar{\mathbf{U}}, \boldsymbol{\lambda}) = \sum_{l=1}^L \alpha_l(\bar{\mathbf{U}}, \boldsymbol{\lambda}) \mathbf{B}_l(\mathbf{X})$$

- Construct reduced basis functions  $\mathbf{B}_l(\mathbf{X})$  from a collection of precomputed stress fields with **proper orthogonal decomposition** (POD)



# Methodology

## Effective Quantities

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

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

Stiffness/Sensitivities depend on derivatives of  $\alpha_l(\bar{\mathbf{F}}, \boldsymbol{\lambda})$

$\Rightarrow$  Construct  $\hat{\alpha}_l(\bar{\mathbf{U}}, \boldsymbol{\lambda})$ ,  $\frac{\partial \hat{\alpha}_l(\bar{\mathbf{U}}, \boldsymbol{\lambda})}{\partial \bar{\mathbf{U}}}$ ,  $\frac{\partial \hat{\alpha}_l(\bar{\mathbf{U}}, \boldsymbol{\lambda})}{\partial \boldsymbol{\lambda}}$  with Gaussian Process Regression

Automatic relevance determination (ARD) squared exponential kernel

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

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

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

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

# Numerical Examples

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

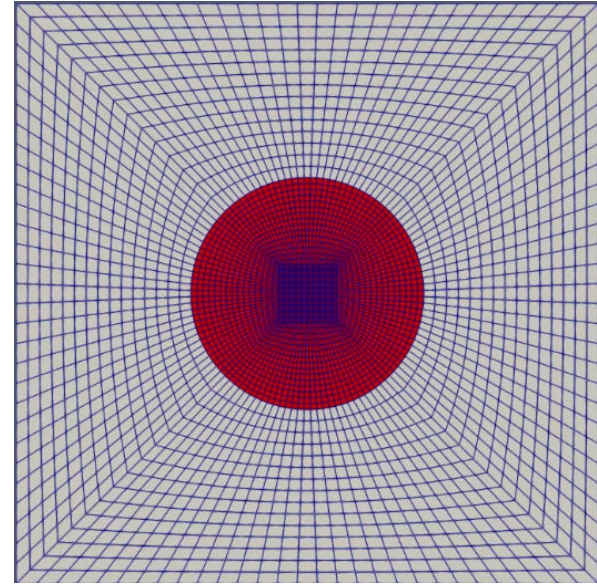
## Fiber reinforced microstructure

- 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  $\bar{\mathbf{U}} - \mathbf{I} \in [-0.3, 0.3]$
- 200 training snapshots (Sobol sequence)
- 500 testing snapshots (uniformly random)
- P-PODGPR Error

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

- Projection Error

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



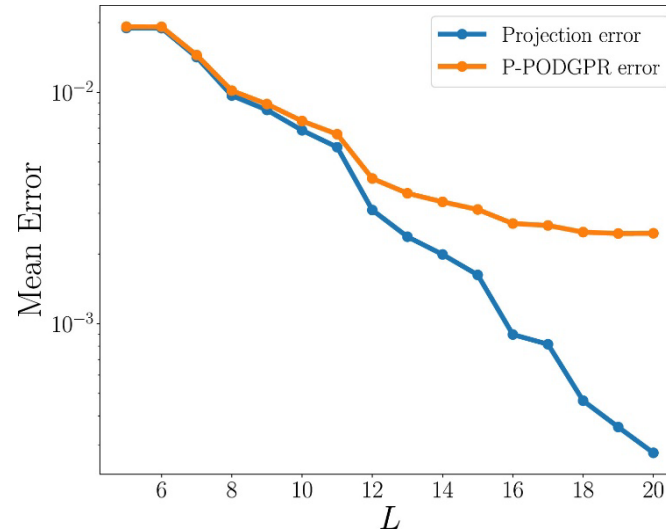
$$W(\mathbf{F}, \boldsymbol{\lambda}) = C_1(\text{Tr}(\mathbf{F}^T \mathbf{F}) - 3 - 2 \ln(\det \mathbf{F})) + D_1(\det \mathbf{F} - 1)^2$$

# Numerical Examples

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

## Fiber reinforced microstructure

Test error of 500 testing snapshots trained with 200 training snapshots



Mean error  $\approx 0.003$

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

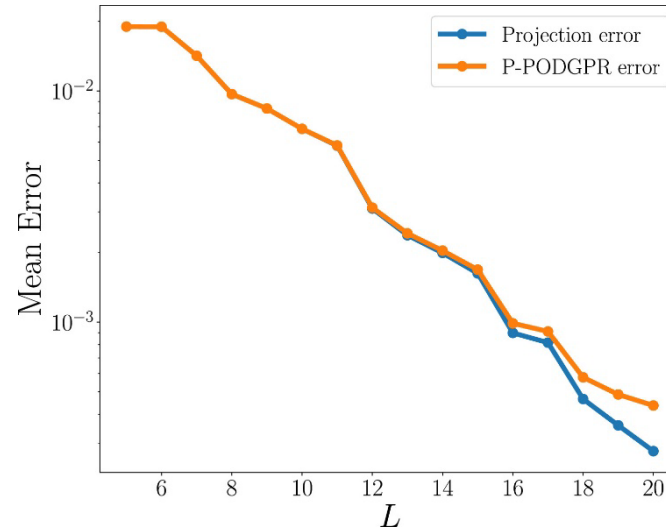
$$\text{Projection Error} \quad \epsilon_{\bar{\mathbf{P}}} := \frac{\|\bar{\mathbf{P}}^{\text{HF}} - \bar{\mathbf{P}}^{\text{RB}}\|_{\text{F}}}{\|\bar{\mathbf{P}}^{\text{HF}}\|_{\text{F}}}$$

# Numerical Examples

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

## Fiber reinforced microstructure

Test error of 500 testing snapshots trained with 500 training snapshots



Mean error  $\approx 0.0004$

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

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

# Numerical Examples

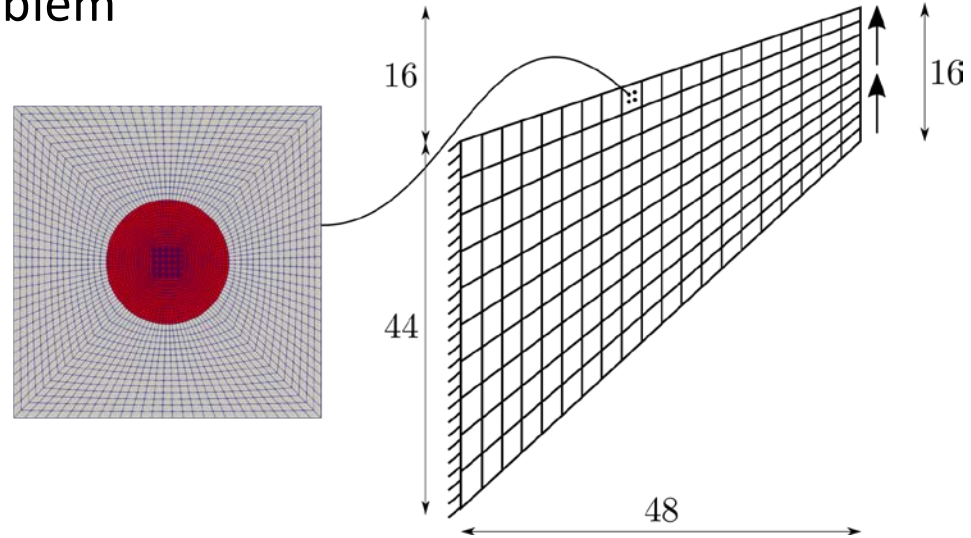
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## 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 stresses

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

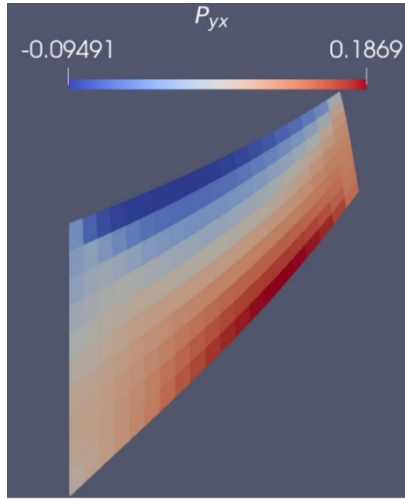
$\langle |P_{yx}^{\text{FE2}}| \rangle$ : Averaged absolute stress



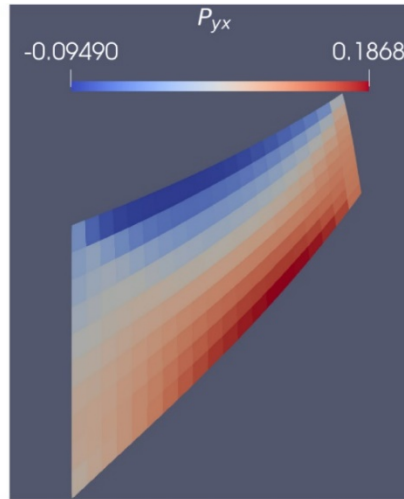
$$W(\mathbf{F}, \lambda) = C_1(\text{Tr}(\mathbf{F}^T \mathbf{F}) - 3 - 2 \ln(\det \mathbf{F})) + D_1(\det \mathbf{F} - 1)^2$$

# Numerical Examples

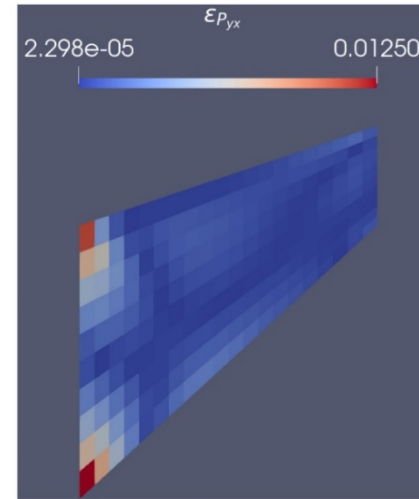
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]



(a)  $FE^2$



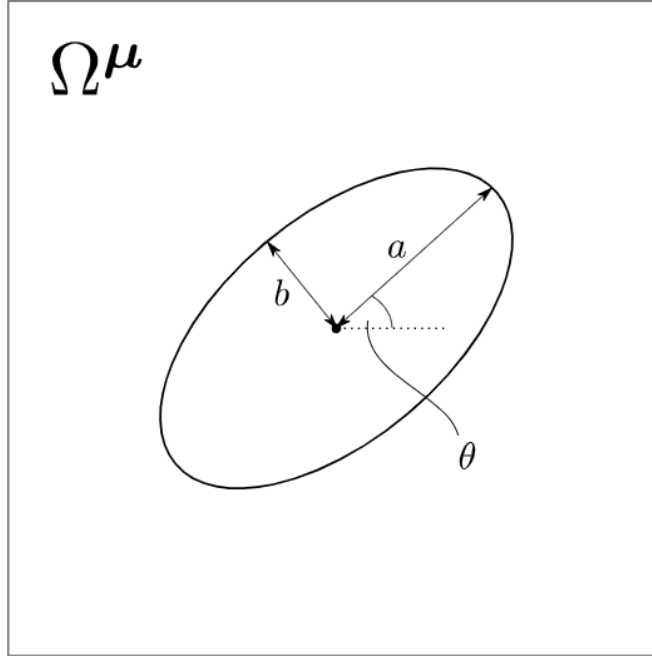
(b) FE with P-PODGPR



(c) Relative error

	$FE^2$	FE with P-PODGPR
Snapshot generation	-	60 min
POD + GPR	-	1 min
Online simulation	4800 min	1 min

# Geometrical Parameters



$a$  : Semi-major axis

$b$  : Semi-minor axis

$\theta$  : Rotation angle

# Geometrical Parameters

Problems:

- Different geometry generally leads to different meshes used  $\rightarrow$  solution for different geometries known at different discrete points  $\rightarrow$  needs interpolation
- Poor performance of POD

Approach:

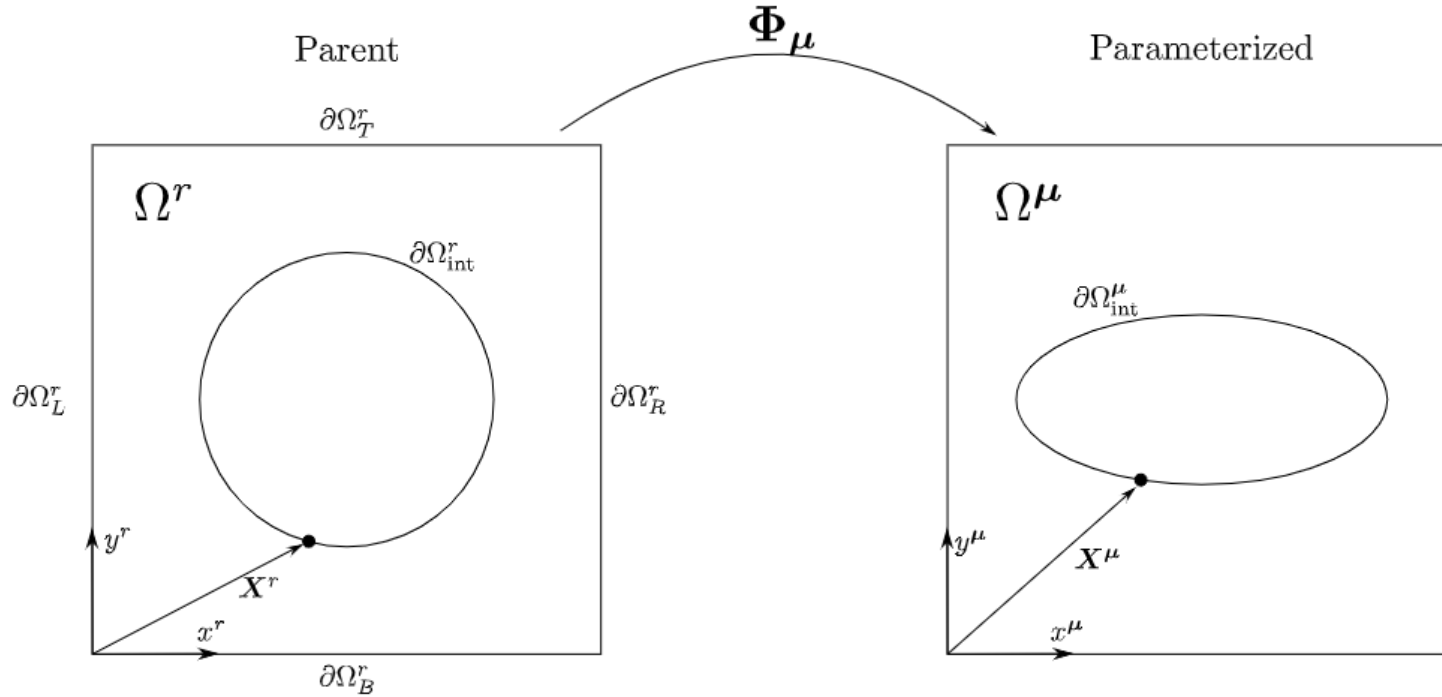
- Transformation of snapshots from a parent domain

$$\Phi_{\mu} : \Omega^r \rightarrow \Omega^{\mu}, X^r \mapsto X^{\mu}$$

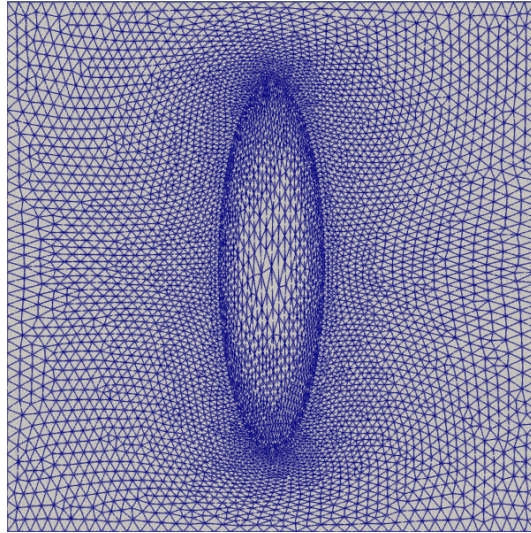
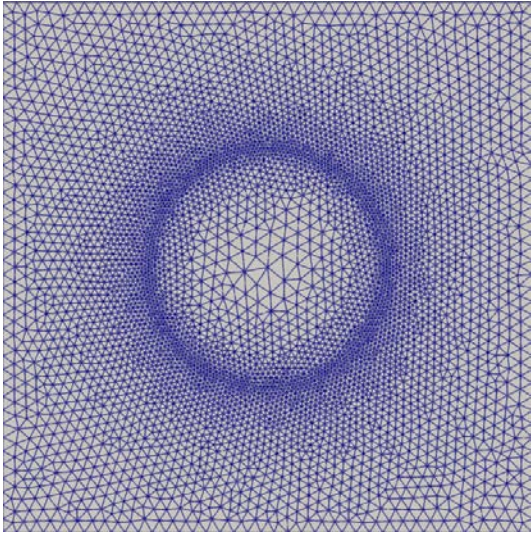
$$P^r(X^r) := P(\Phi_{\mu}(X^r))$$



# Geometrical Parameters



# Geometrical Parameters



Fixing loading parameters and semi-major and minor axis, varying rotation angle

## Summary

- Approximation of stress field based on proper orthogonal decomposition and Gaussian process regression
- Validated on 2D composite microstructure and a two-scale application
- High accuracy and online speedup
- Extension to geometrically parameterized microstructures

## Outlook

- Two-scale optimization with surrogate model
- Reduce number of samples needed for training
- More complicated material models (Plasticity, Damage)

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**Acknowledgments:** This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 818473).

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# Methodology

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

## Proper Orthogonal Decomposition (POD)

1. Generate samples  $\left[ (\bar{\mathbf{F}}^{(1)}, \boldsymbol{\lambda}^{(1)}), (\bar{\mathbf{F}}^{(2)}, \boldsymbol{\lambda}^{(2)}), \dots, (\bar{\mathbf{F}}^{(N_{\text{pod}})}, \boldsymbol{\lambda}^{(N_{\text{pod}})}) \right]$
2. Compute and collect stress snapshots  $\mathbf{S} = [\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \dots, \mathbf{P}^{(N_{\text{pod}})}]$
3. Compute correlation matrix

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

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

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

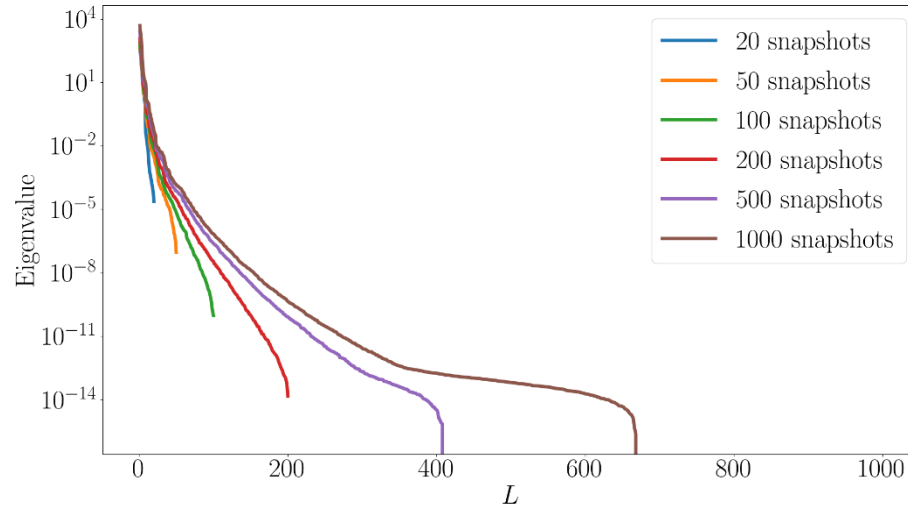
$$\Rightarrow \mathbf{P}^{\text{RB}}(\mathbf{X}, \bar{\mathbf{F}}, \boldsymbol{\lambda}) = \sum_{l=1}^L \alpha_l(\bar{\mathbf{F}}, \boldsymbol{\lambda}) \mathbf{B}_l(\mathbf{X})$$

# Numerical Examples

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

## Fiber reinforced microstructure

POD for different numbers of training snapshots



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

# 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]

[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  $k_\theta(\mathbf{X}, \mathbf{X}')$

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

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

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

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

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

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



# Numerical Examples

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

## Fiber reinforced microstructure

- Comparison with a neural network (Multilayer Perceptron) that is trained with pairs of  $\{(\bar{\mathbf{F}}, \boldsymbol{\lambda})^{(i)}, \bar{\mathbf{P}}^{(i)}\}_{i=1}^N$  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	$\epsilon_{\mathbf{P}}^{\text{mean}}$	$\epsilon_{\mathbf{P}}^{\text{max}}$
$N_h = 1, N_n = 20$	$1.7 \times 10^{-6}$	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

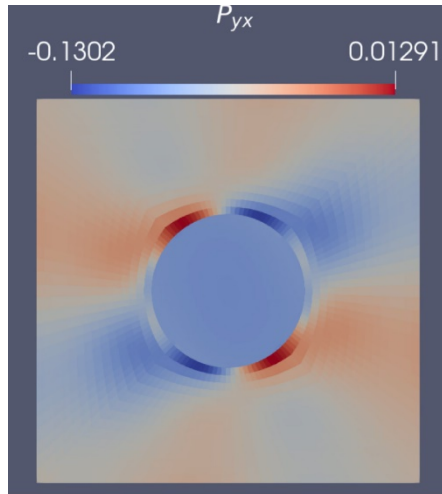
⇒ P-PODGPR outperforms all neural networks

# Numerical Examples

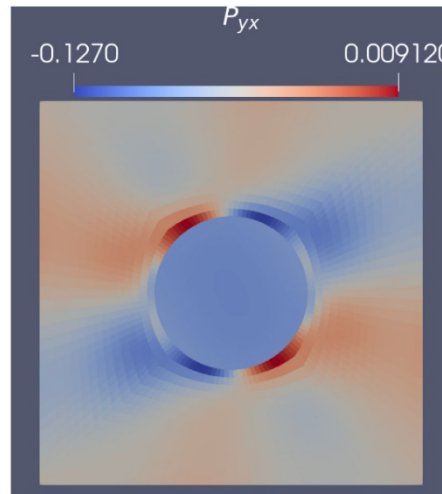
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

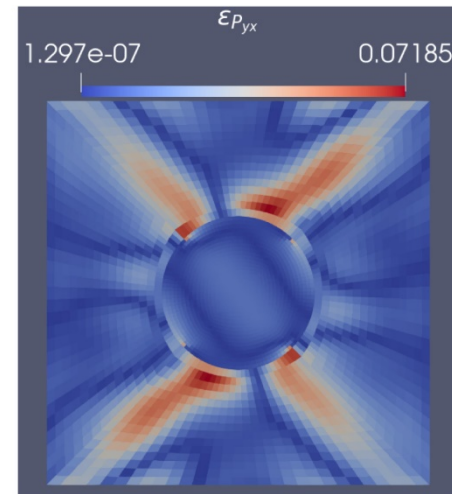
Microscopic stress component  $P_{yx}$  at point A



(a)  $FE^2$



(b) FE with P-PODGPR



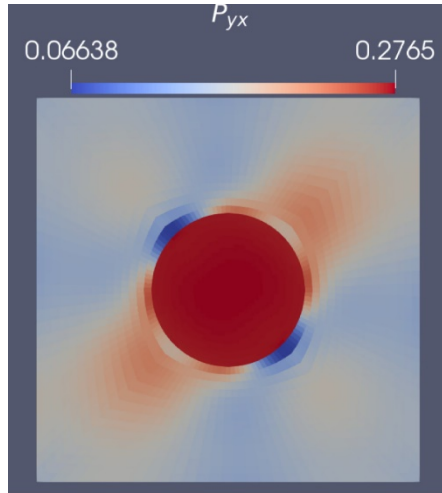
(c) Relative error

# Numerical Examples

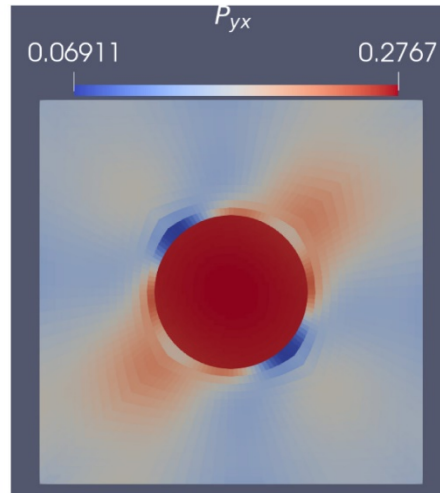
[Guo, T., Rokoš, O., and Veroy, K., 2021, CMAME 384]

## Two-scale Cook's membrane problem

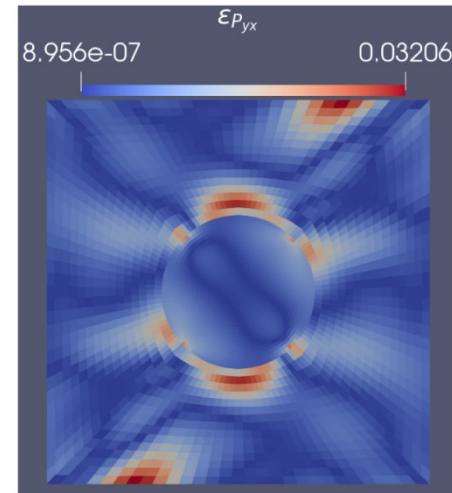
Microscopic stress component  $P_{yx}$  at point B



(a)  $FE^2$



(b) FE with P-PODGPR



(c) Relative error

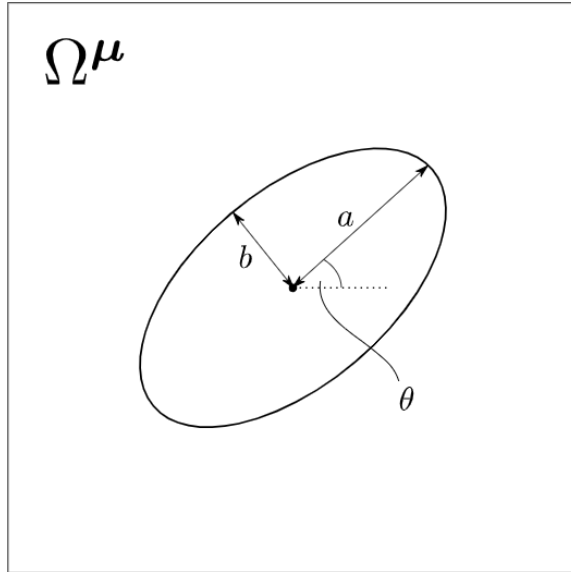
# Current Research: Geometrical Parameters

## Related Works

- Analytical Transformation
  - [Moreau, A., et al., 2021, Acta Mechanica]
  - [Rozza, G., Huynh, D.B.P., Patera, A.T., 2008, Arch. Comput. Meth Eng.]
- Shape Deformation Techniques
  - [Sieger, D., Menzel, S., Botsch, M., 2015, Springer]
  - [Rozza, G., et al., 2020, De Gruyter]
- Image Registration Method
  - [Taddei, T., 2020, SIAM SC]

# Current Research: Geometrical Parameters

## Example: Rotating Elliptical Fiber



### Auxiliary Problem

$$\begin{aligned} \text{Div}(\mathbb{C} : \nabla^s d) &= 0 && \text{on } \Omega^r, \\ d &= 0 && \text{on } \partial\Omega^r, \\ d &= \mathbf{X}^\mu - \mathbf{X}^r && \text{on } \partial\Omega_{\text{interface}}^r; \end{aligned}$$

Interface deformation is known and can be prescribed!

$$\mathbf{X}^\mu = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} a/r & 0 \\ 0 & b/r \end{bmatrix} \begin{pmatrix} \tilde{r} \cos(\tilde{\theta} - \theta) \\ \tilde{r} \sin(\tilde{\theta} - \theta) \end{pmatrix} \quad \begin{aligned} \tilde{r} &= \sqrt{\mathbf{X}^{r^T} \mathbf{X}^r} \\ \tilde{\theta} &= \arctan2(y^r, x^r) \end{aligned}$$

3 geometrical parameters + 4 loading parameters

# Current Research: Geometrical Parameters

Problems:

- Different meshes used for different snapshots
- Solutions do not lie in linear subspace  $\rightarrow$  poor performance of POD

Solution:

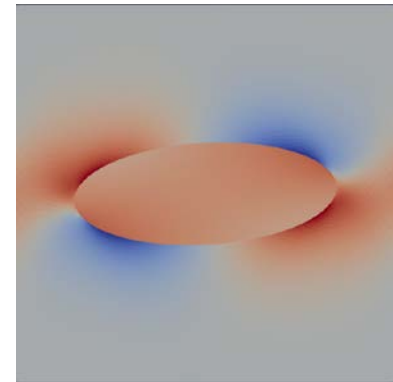
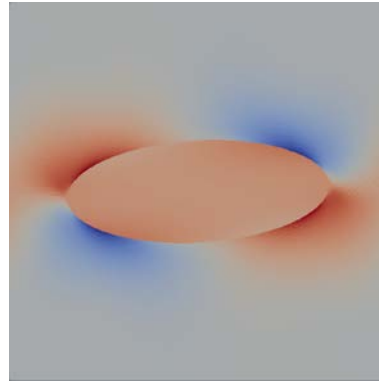
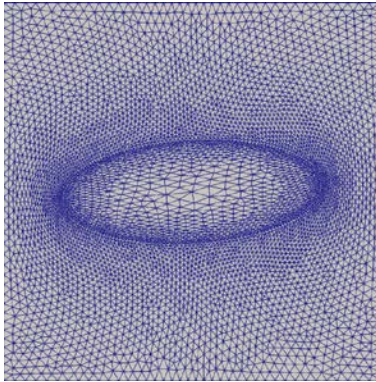
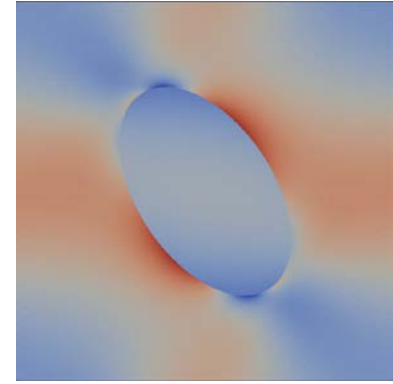
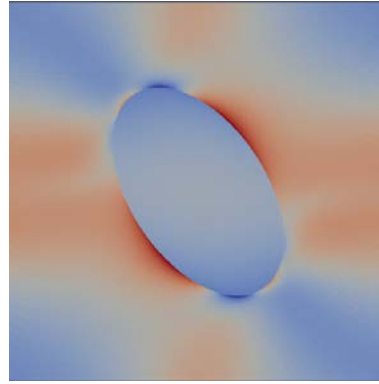
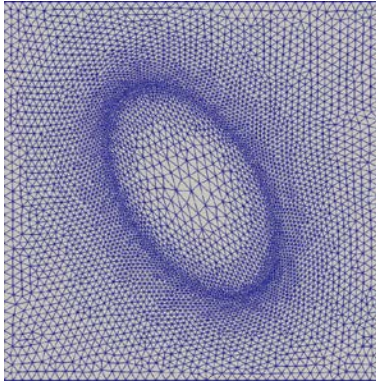
- Transformation of snapshots onto a reference domain

$$\Phi_\mu : \Omega^r \rightarrow \Omega^\mu, X^r \mapsto X^\mu \quad P(X^\mu) = P(\Phi_\mu(X^r)) =: P^r(X^r)$$

- Effective stress can be obtained with

$$\begin{aligned} \bar{P}(\bar{F}, \lambda, \mu) &= |\Omega^\mu|^{-1} \int_{\Omega^\mu} P(X^\mu; \bar{F}, \lambda, \mu) dX^\mu \\ &= |\Omega^\mu|^{-1} \int_{\Omega^r} P^r(X^r; \bar{F}, \lambda, \mu) |\det D\Phi_\mu| dX^r \end{aligned}$$

# Geometrical Parameters



# Problem Statement

Linear Momentum Balance  $\bar{\mathbf{u}}(\bar{\mathbf{X}})$

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

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

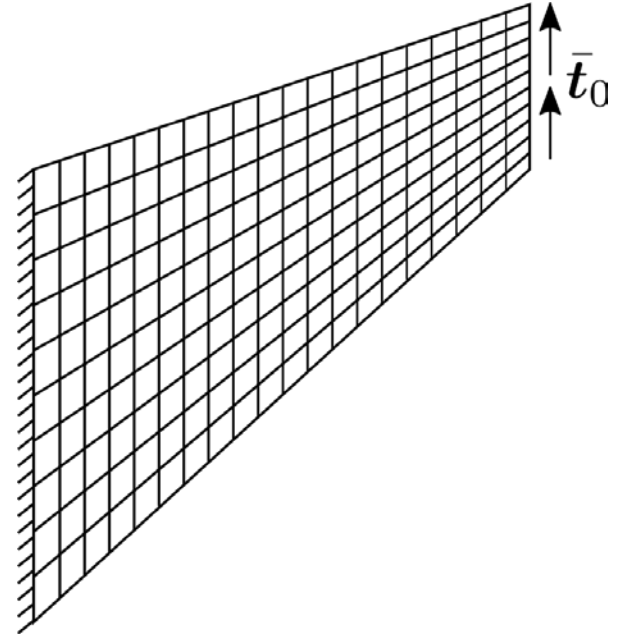
$$\bar{\mathbf{u}} = \bar{\mathbf{u}}_0 \quad \text{on } \partial \bar{\Omega}^D,$$

$\bar{\mathbf{P}}$  : Stress Tensor

$\bar{\mathbf{u}}$  : Displacement

$\bar{\mathbf{F}}$  : Deformation Gradient

$\mu$  : Parameters



Constitutive Model

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

Highly **nonlinear** operator

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

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

Often not interpretable  
parameters  $\mu$

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