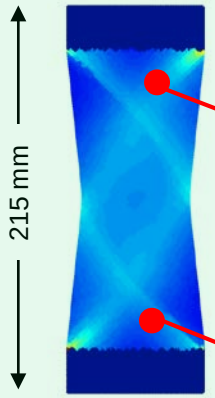
Nested Multiscale Simulations

(1) Woven Composite at Macroscale



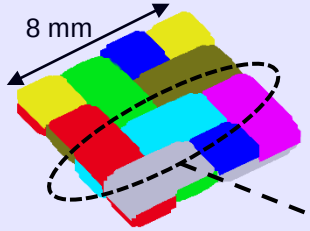
i^{th} IP

j^{th} IP

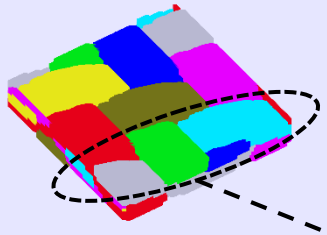
$v_f = 65\%$

15,000 IPs

(2) Cured Woven-RVE at Mesoscale

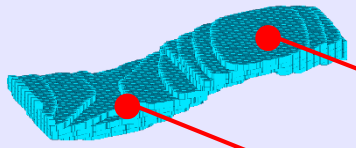


$\alpha = 90°$
$v_f = 62\%$



$\alpha = 80°$
$v_f = 68\%$

640,000 IPs



80,000 IPs

* Resin not shown

- Integration points (IPs) are structures at finer scales.

α: Yarn angle

v_f: Avg. fiber volume fraction

(3) Cured UD-RVE at Microscale

i^{th} IP

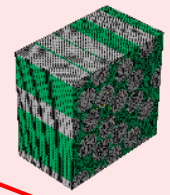
j^{th} IP

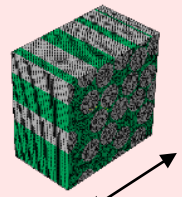
$v_f = 60\%$

$v_f = 65\%$

i^{th} IP

j^{th} IP

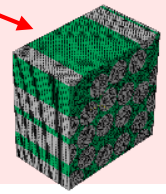


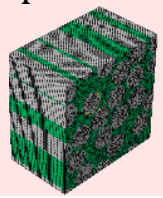


10 μm

$v_f = 64\%$

$v_f = 70\%$





900,000 IPs

Prior Works:

- Random process based UQ in a *single* length-scale
- Neglecting *spatial & part-to-part* variations

Our Approach For UQ & UP in Multiscale Simulations

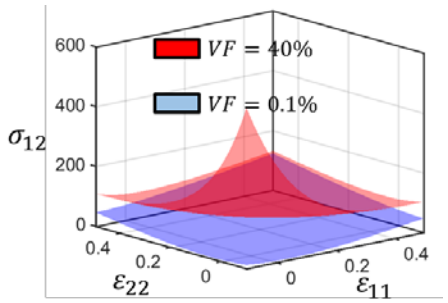
- Modeling uncertainties sources and their spatial variations via spatial random processes (SRPs)
- Coupling SRPs across length-scales via top-down sampling
- Creating metamodels of homogenized constitutive relations w microstructure variations

Managing Complexity – On-the-fly Machine Learning

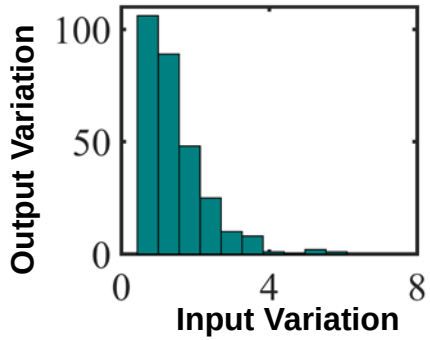
Homogenization Speed-up

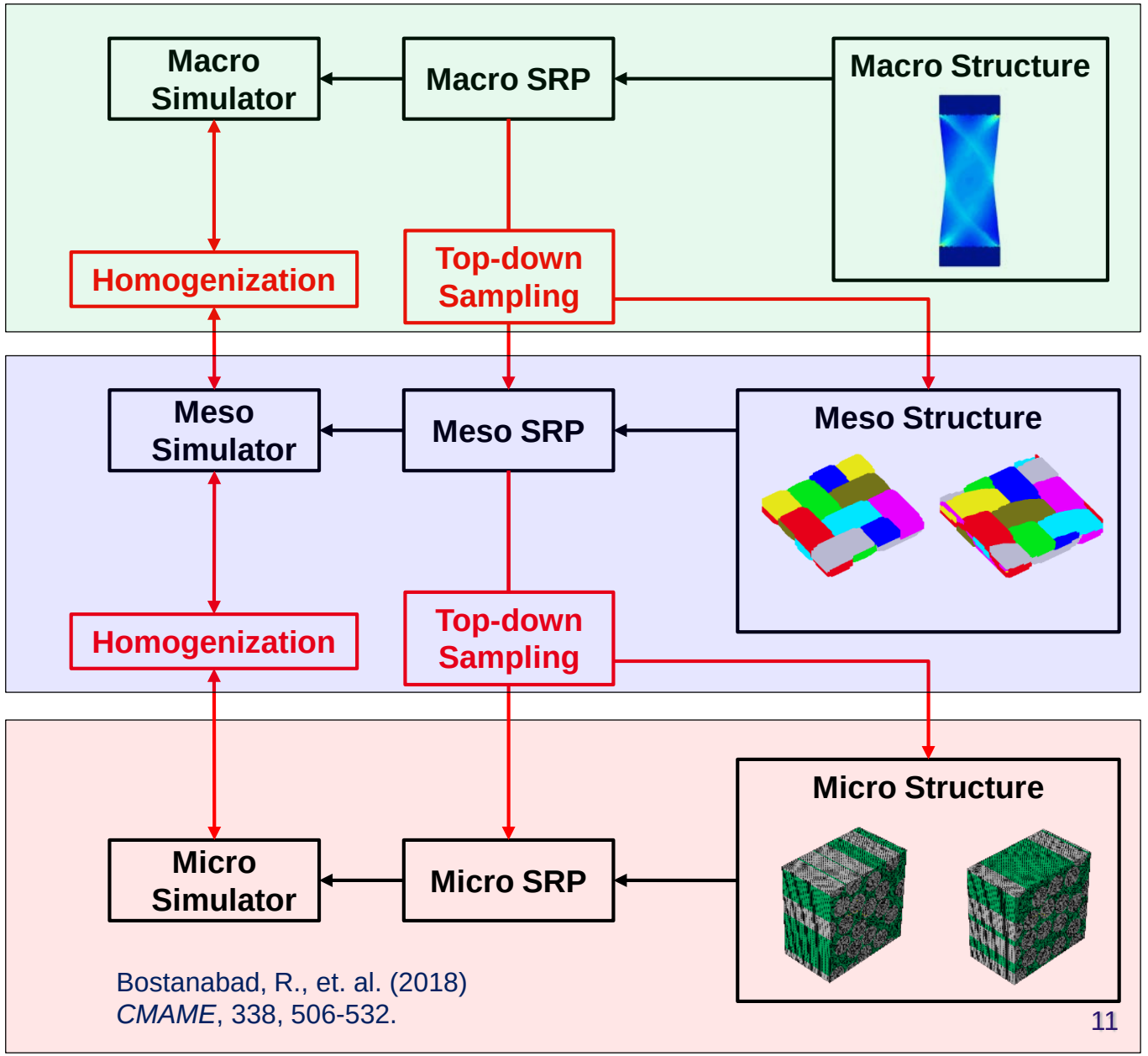
Sampling Dimension Reduction

Metamodeling



Sensitivity Analysis





Bostanabad, R., et. al. (2018) *CMAME*, 338, 506-532.

Multi-Response Gaussian Processes (MRGPs) for Quantifying Correlated Uncertain Sources

- ❑ Only need mean and covariance functions.
- ❑ Single response Gaussian processes:

$$\boldsymbol{y} \sim GP\left(m(\cdot), \sigma^2 \boldsymbol{r}(\cdot,\cdot)\right)$$

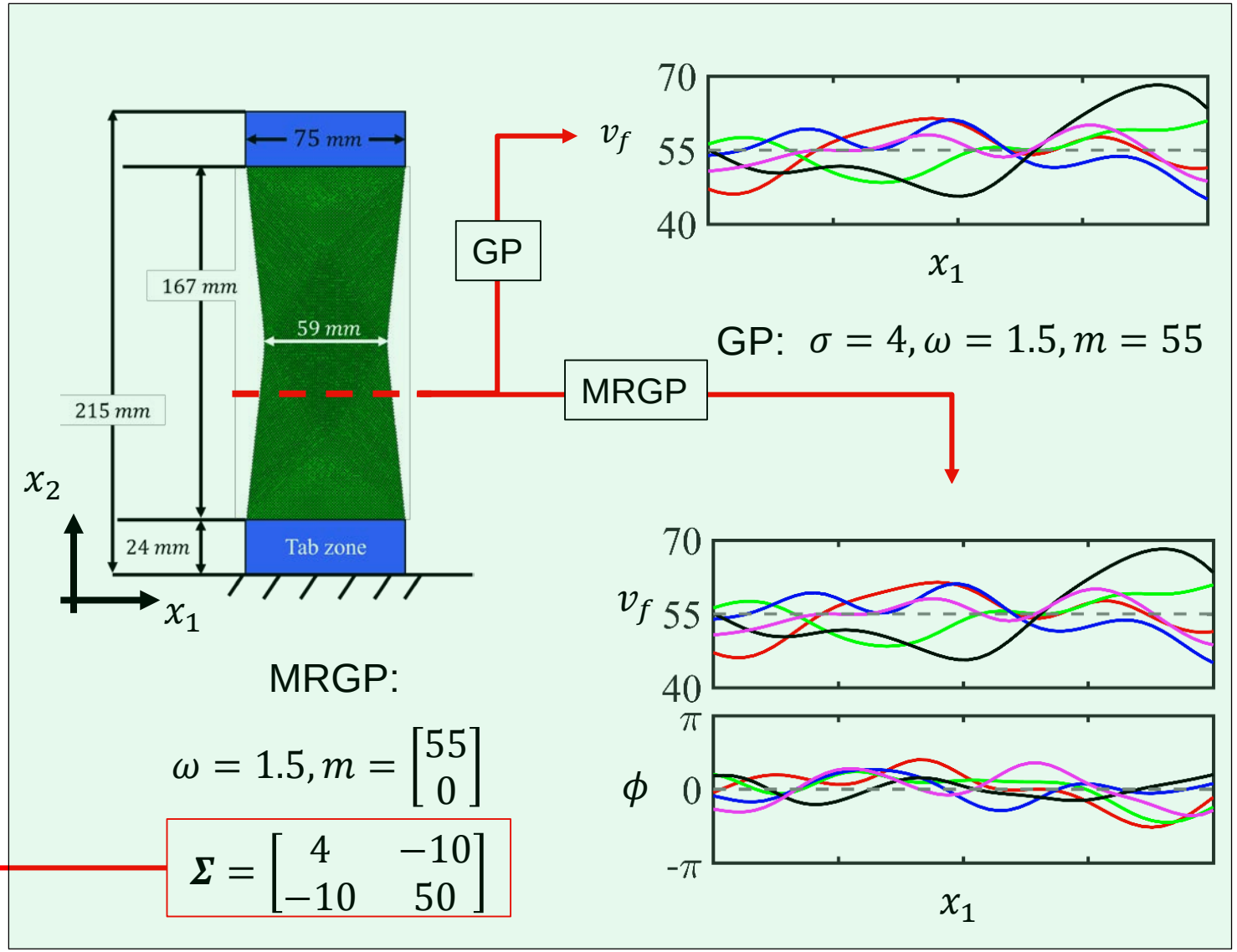
Mean Function **Covariance Function**

$$r(\boldsymbol{x}, \boldsymbol{x}') = e^{-\sum_{i=1}^{p} 10^{\omega_i}\left(x_i - x_i'\right)^2}$$

- ❑ Multi-response Gaussian process (MRGP):

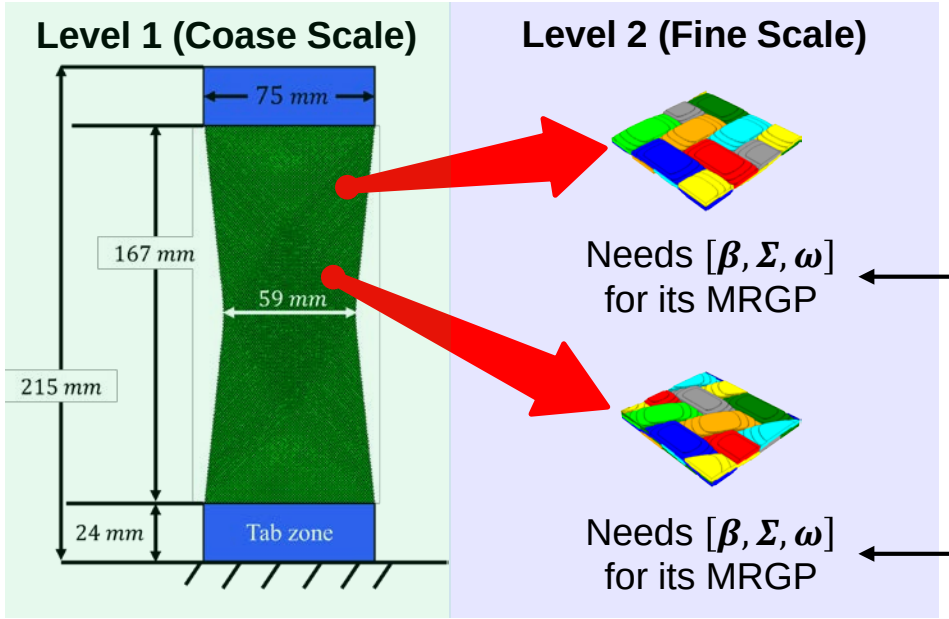
$$\boldsymbol{Y} \sim MRGP(\boldsymbol{m}(\cdot), \boldsymbol{\Sigma} \otimes \boldsymbol{r}(\cdot,\cdot))$$

- Captures the **between-response correlations** & **variations around the means**.



Top-down Sampling

- **Hyperparameters** of the MRGP at the **higher** scale are considered as the **responses** of the MRGP at the **lower** scale.



Macroscale MRGP

$$Y^1 \sim MRGP\left(\beta^1, \Sigma^1 \otimes r^1(\cdot,\cdot)\right)$$

Realization 1

$$\left[\beta^2, \Sigma^2, r^2\right] \longleftarrow y_1^1$$

Realization 2

$$\left[\beta^2, \Sigma^2, r^2\right] \longleftarrow y_2^1$$

- Hierarchy of random fields.
- Non-stationary random field at the fine scale.
- No limit on the number of levels/scales.

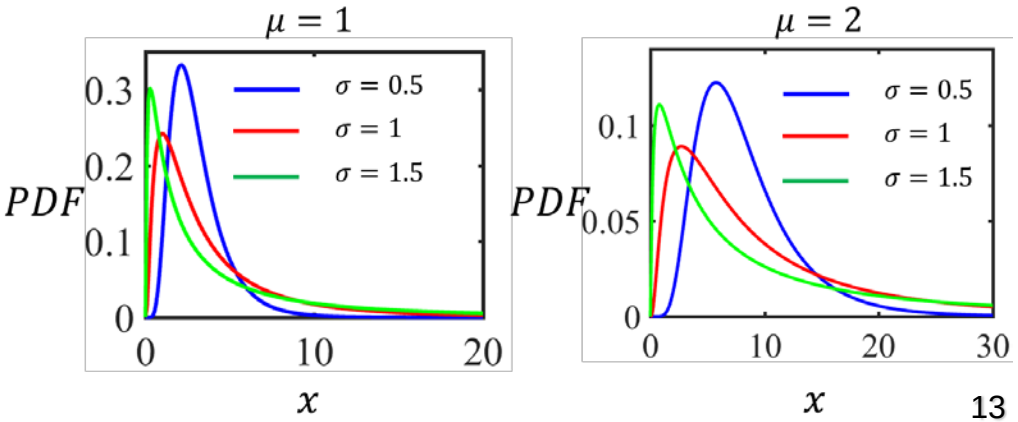
- **Superscripts** → Level
- **Subscripts** → Counter (e.g., for realization)

Transformation: required if the underlying distribution is not normal.

- For Y normal and $X = \exp(Y)$:

$$\sigma_Y^2 = \ln\left(1 + \frac{\sigma_X^2}{\mu_X^2}\right)$$

$$\mu_Y = \ln\left(\frac{\mu_X}{\sqrt{1 + \frac{\sigma_X^2}{\mu_X^2}}}\right)$$



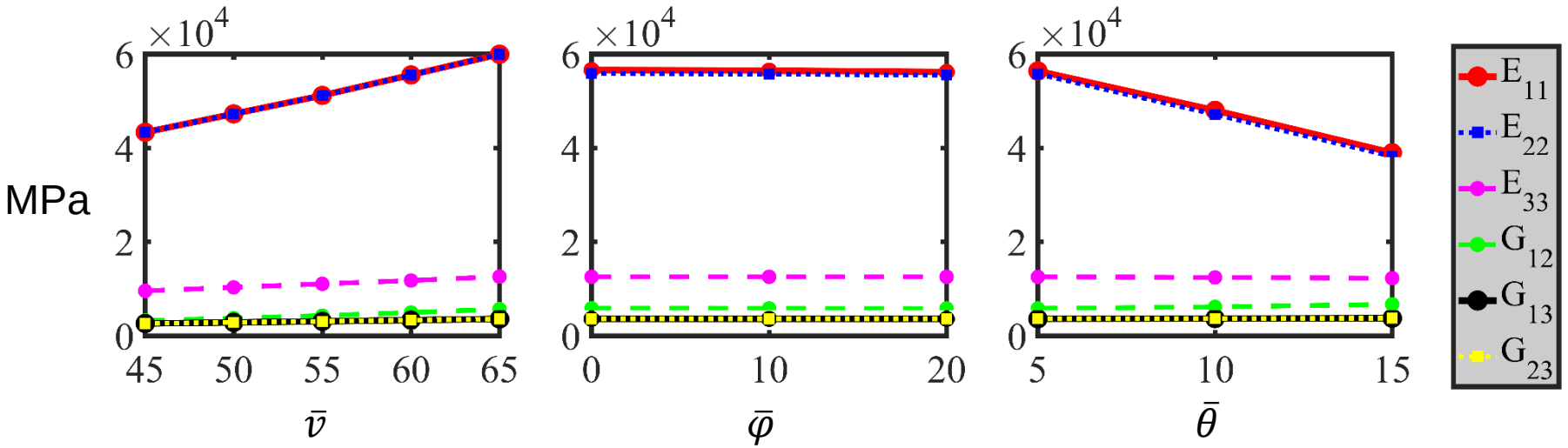
Sensitivity Analysis of Cascaded Effects to the Mesoscale: Moduli

1. Fiber volume fraction:

- The **average** ($\bar{v}$) is important.
- **Spatial variations** are **not** important.

2. Misalignment angle:

- The average zenith angle ($\bar{\theta}$) is important.
- Spatial variations of θ are **not** important.
- The average and spatial variations of azimuth angle (φ) are **not** important.



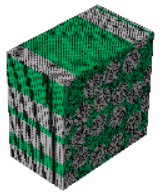
NOTE: Each point in the figure is averaged over 30 simulations

❑ **Sensitivity analyses for dimension reduction:** Identify the hyperparameters that affect the homogenized response of a woven RVE:

- $\boldsymbol{\beta}$ important → Mean values important
- $\boldsymbol{\Sigma}$ or $\boldsymbol{\omega}$ important → Spatial variations important

Microscale & Mesoscale Metamodels

Micro: Predicting the stiffness matrix of a UD- RVE for any values of ${}^3\bar{v}, E_f, E_m$.

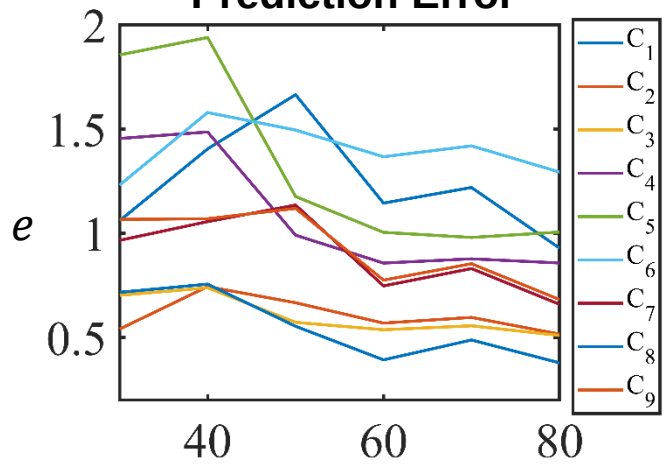


- **MRGP training:** 30 to 80 samples
- **Validation:** 20 samples

Stiffness Matrix of UD-RVE

$$ {}^3\overline{\boldsymbol{C}} = \begin{bmatrix} C_1 & C_7 & C_9 & 0 & 0 & 0 \\ C_7 & C_2 & C_8 & 0 & 0 & 0 \\ C_9 & C_8 & C_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & C_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_6 \end{bmatrix} $$

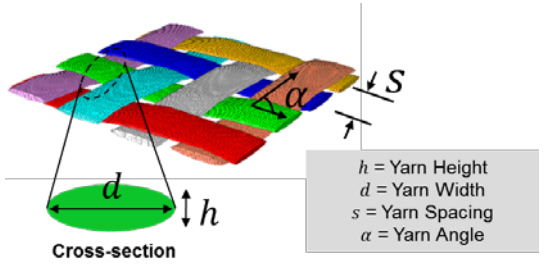
Prediction Error



Size of the training dataset

Meso: Predicting the stiffness matrix of a woven-RVE for any values of α, ${}^2\bar{v}$ and ${}^2\bar{\theta}$.

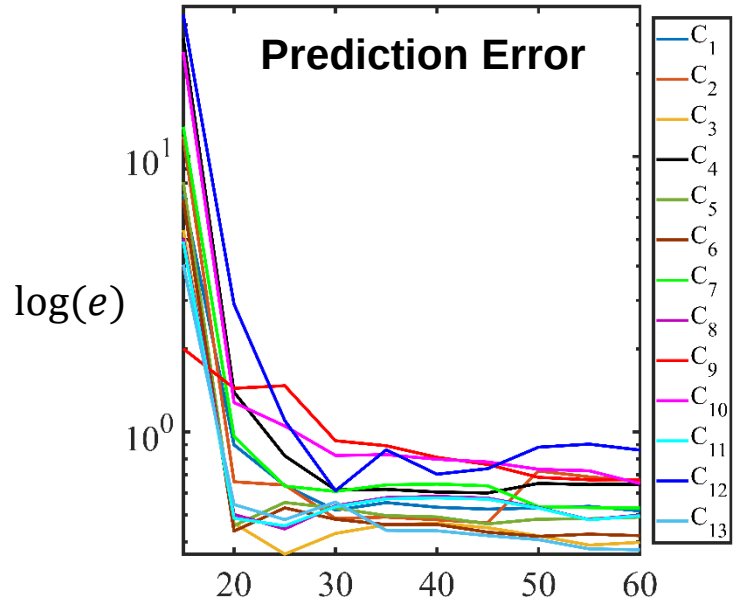
- **MRGP training:** 10 to 60 samples
- **Validation:** 20 samples



Stiffness Matrix of the Woven RVE

$$ {}^2\overline{\boldsymbol{C}} = \begin{bmatrix} C_1 & C_7 & C_{11} & C_{13} & 0 & 0 \\ C_7 & C_2 & C_8 & C_{12} & 0 & 0 \\ C_{11} & C_8 & C_3 & C_9 & 0 & 0 \\ C_{13} & C_{12} & C_9 & C_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_5 & C_{10} \\ 0 & 0 & 0 & 0 & C_{10} & C_6 \end{bmatrix} $$

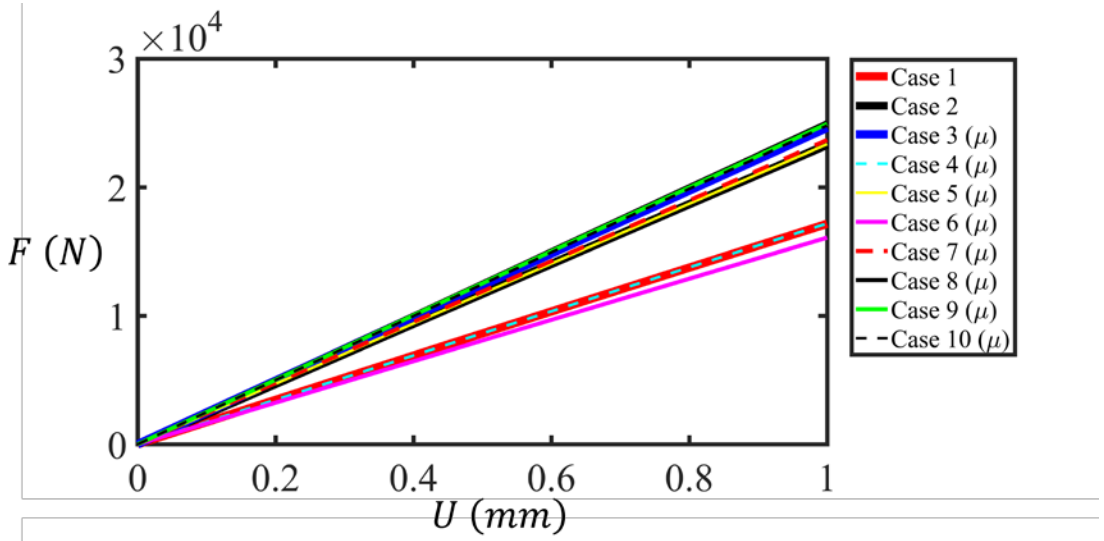
$$ e = 100 \sqrt{\frac{1}{20} \sum_{i=1}^{20} \left(1 - \frac{\hat{y}}{y}\right)^2} \ \% $$

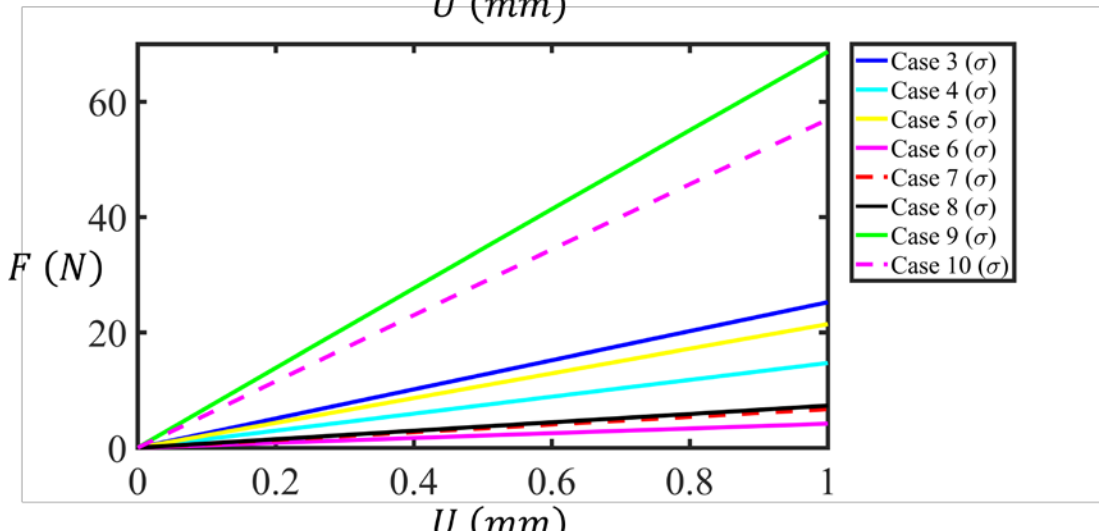


Size of the training dataset

Uncertainty Impacts at the Macroscale

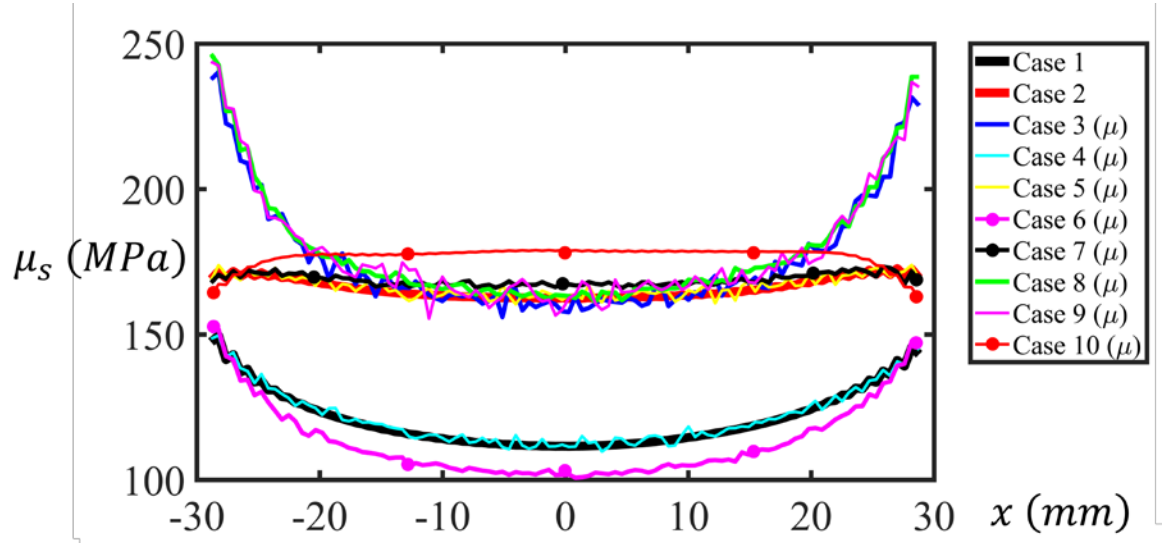
Effect on global response: Reaction force (17%) affected by the spatial variations.

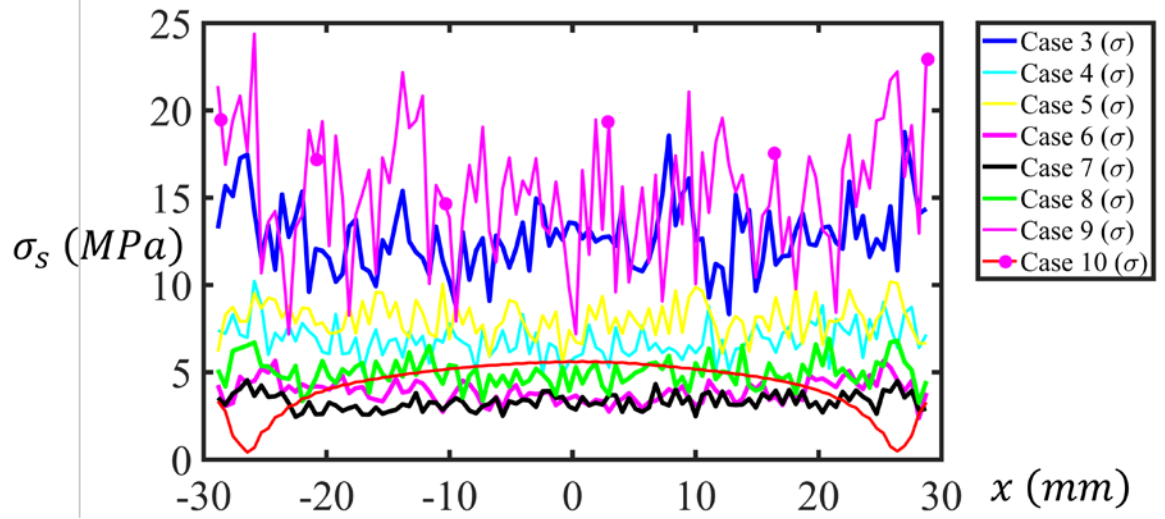




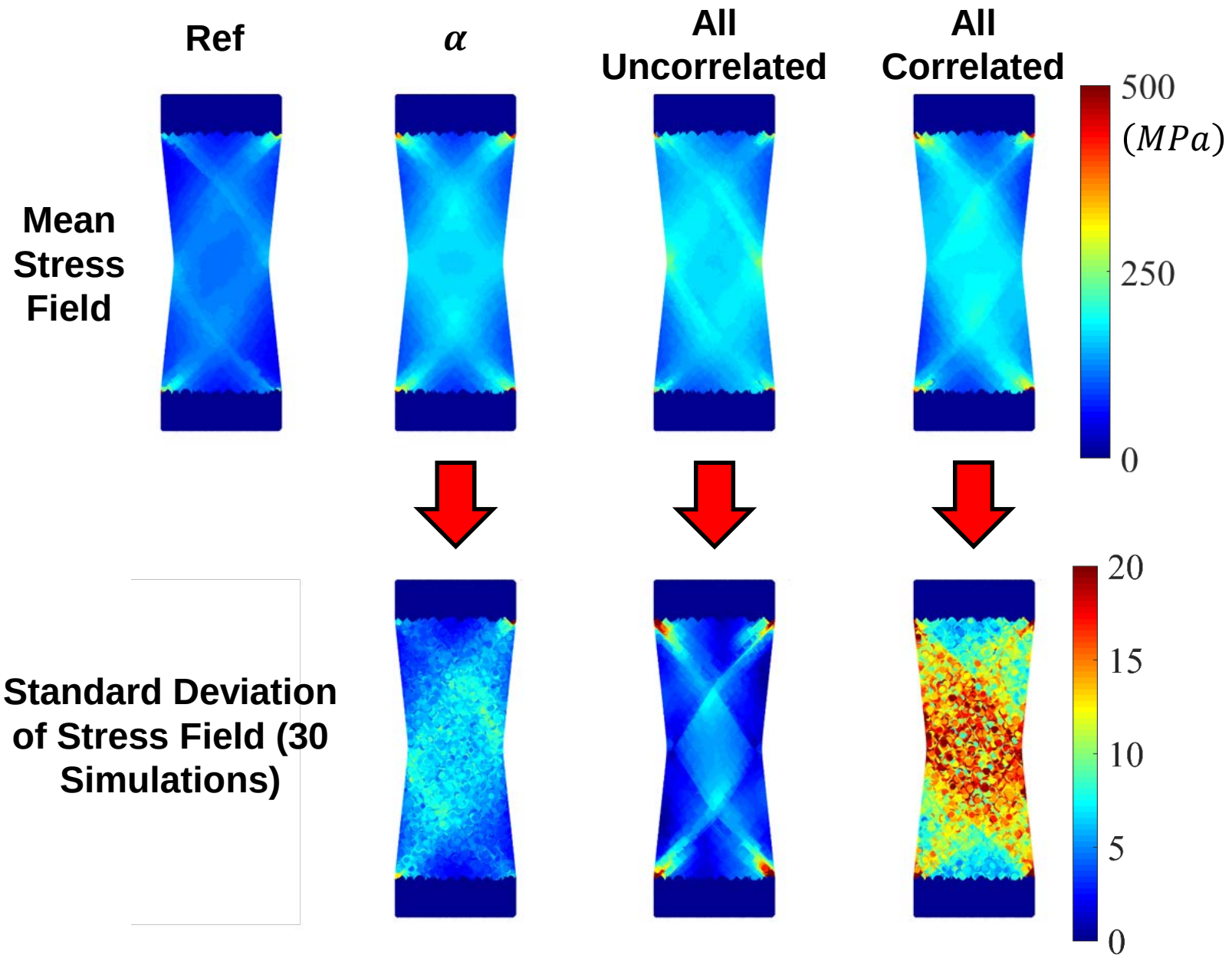
Effect on local stress in the mid-section

- The coefficient of variation $\frac{60}{600} \times 100 = 10\%$.





Comparison of Macroscale Stress Fields



- Ref: Reference solution without any spatial variations.
- Spatial variations of yarn angle are more important than the other parameters.
- Correlated spatial variations result in higher stress values.
- The only difference between the cases is spatial variations (i.e., the averages are the same).

Remarks on Our Approach

- **Non-intrusive:** No need to edit the finite element codes
- **Uncertainty Sources:** Accounting for multi-response non-stationary uncertain sources
- **Multiscale:** Effect of micro and meso uncertainties on macro response
- **Physical insights:** MRGP hyperparameters can be directly linked to physical parameters and physical constraints
- **Impact:** Uncertain impact will be more critical for nonlinear behavior