Learning Constitutive Models in Multiscale Modeling of Materials

4TU.HTM WORKSHOP 2021, 23-06-2021

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Outline

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

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).
Problem Statement

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

$$\text{Div} \tilde{P}(\tilde{u}) = 0 \quad \text{on } \tilde{\Omega},$$
$$\tilde{P} \tilde{N} = \tilde{t}_0 \quad \text{on } \partial \tilde{\Omega}^N,$$
$$\tilde{u} = \tilde{u}_0 \quad \text{on } \partial \tilde{\Omega}^D,$$

Constitutive Model

$$\tilde{P} = \tilde{P}(\tilde{F}, \mu)$$

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

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

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

**Microscopic Problem:** Find $u(X)$

\[
\text{Div} \, P(u) = 0 \quad \text{on} \quad \Omega \\
u = (\bar{F} - I)X + w(X)
\]

(mean \hspace{1cm} fluctuation)

**Neo-Hookean material**

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

\[
P(F, \mu) = \frac{\partial W}{\partial F} \quad \bar{F} \quad \text{loading: macroscopic deformation gradient}
\]

\[
A(F, \mu) = \frac{\partial P}{\partial F} \quad \mu \quad \text{parameters: material & geometry}
\]

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

Scale Coupling

Hill-Mandel Condition

\[ \langle P : \delta F \rangle = \bar{P} : \delta \bar{F} \]

\[ w = 0 \quad \text{on } \partial \Omega \quad \text{(KBC)} \]

\[ w \text{ periodic on } \partial \Omega \quad \text{(PBC)} \]

Effective Quantities

\[ \bar{P} = \langle P \rangle \]

\[ \bar{A} \neq \langle A \rangle \]

\[ \text{Macro scale} \]

\[ \nabla \bar{P} + \bar{B} = 0 \]

\[ \text{(c) } \bar{P}, \bar{A} \]

\[ \text{(a) } \bar{F} \]

\[ \text{(b) Microscale} \]

\[ \nabla P = 0 \]

[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

\[ f(\Phi \alpha) = 0 \]

Need hyperreduction!

\[ \Phi^T Df|_{\Phi \alpha^k} \Phi \Delta \alpha = -\Phi^T f(\Phi \alpha^k) \]

\[ \alpha^{k+1} = \alpha^k + \Delta \alpha \]

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

Non-Intrusive RB Method

Approximate displacement field

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

Instead of solving reduced system, perform a regression to obtain

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

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

[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]
Methodology

Non-Intrusive RB Method

Approximate displacement field

\[ u(x, \bar{F}, \mu) \approx \sum_{l=1}^{L} \alpha_l(\bar{F}, \mu) \Phi_l(x) = \Phi \alpha \quad \text{with} \quad \Phi(x) \quad \text{RB basis functions} \]

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!

\[ P(x, \bar{F}, \mu) \approx \sum_{l=1}^{L} \alpha_l(\bar{F}, \mu) B_l(x) \]
Methodology

Proper Orthogonal Decomposition (POD)

1. Collect stress snapshots

   \[ S = \left[ P^{(1)}, P^{(2)}, \ldots, P^{(N_{pod})} \right] \]

2. Compute correlation matrix

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

3. Compute the eigenvalues \( \lambda_l \) and eigenvectors \( v_l \) of \( C \)

4. Compute the basis functions

   \[ B_l = \frac{1}{\sqrt{\lambda_l}} Sv_l \]

   \[ (B_i, B_j)_{L^2(\Omega)} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \]

   \[ \Rightarrow P^{RB}(X, \bar{F}, \mu) = \sum_{l=1}^{L} \alpha_l(\bar{F}, \mu) B_l(X) \]

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

Effective Quantities

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

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

Sensitivities

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

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

\[ \int_\Omega B_l(X) dV \text{ can be computed offline!} \]
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

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

\[
\begin{align*}
    f^*(\mathbf{X}, \mathbf{y}) &\sim \mathcal{GP}(m^*, k^*), \\
    m^*(\mathbf{x}) &= k_{\theta}(\mathbf{X}, \mathbf{x})^T k_{\theta}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{y}(\mathbf{X}), \\
    k^*(\mathbf{x}, \mathbf{x}') &= k_{\theta}(\mathbf{x}, \mathbf{x}') - k_{\theta}(\mathbf{X}, \mathbf{x})^T k_{\theta}(\mathbf{X}, \mathbf{X})^{-1} k_{\theta}(\mathbf{X}, \mathbf{x}')
\end{align*}
\]

where

\[
\begin{align*}
    k_{\theta}(\mathbf{X}, \mathbf{x}) &= [k_{\theta}(\mathbf{X}^{(1)}, \mathbf{x}), k_{\theta}(\mathbf{X}^{(2)}, \mathbf{x}), \ldots, k_{\theta}(\mathbf{X}^{(N)}, \mathbf{x})]^T \\
    k_{\theta}(\mathbf{X}, \mathbf{X}) &= [k_{\theta}(\mathbf{X}^{(i)}, \mathbf{X}^{(j)})]_{i,j=1}^{N} \\
    \mathbf{y}(\mathbf{X}) &= [f(\mathbf{X}^{(1)}), f(\mathbf{X}^{(2)}), \ldots, f(\mathbf{X}^{(N)})]^T
\end{align*}
\]

[Guo, M. and Hesthaven, J.S., 2018, CMAME 341]
[Rasmussen, C.E., 2003, Summer school on machine learning]
Numerical Examples

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 \( \ddot{U} - I \in [-0.3, 0.3] \)
- 500 training snapshots (Sobol sequence)
- 1000 testing snapshots (uniformly random)
- P-PODGPR Error
  \[
  \epsilon_{P} := \frac{\| \bar{P}_{HF} - \bar{P}_{RB} \|_F}{\| \bar{P}_{HF} \|_F}
  \]
- Projection Error
  \[
  \epsilon_{P} := \frac{\| \bar{P}_{HF} - \bar{P}_{RB} \|_F}{\| \bar{P}_{HF} \|_F}
  \]

\[
W(F, \mu) = C_1(Tr(F^T F) - 3 - 2 \ln (\det F)) + D_1(\det F - 1)^2
\]

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

Fiber reinforced microstructure

POD for different numbers of training snapshots

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

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

Fiber reinforced microstructure

Test error in effective stress for 200 training snapshots

Mean error \( \approx 0.003 \)

Max error \( \approx 0.011 \)
Numerical Examples

Fiber reinforced microstructure

Test error in effective stress for 500 training snapshots

Mean error $\approx 0.0004$

Max error $\approx 0.01$

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

Fiber reinforced microstructure

- Comparison with a neural network (Multilayer Perceptron) that is trained with pairs of \( \{U^{(i)}, P^{(i)}\}_{i=1}^{N} \) 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

<table>
<thead>
<tr>
<th>Architecture</th>
<th>Validation Loss</th>
<th>( \epsilon_p^{\text{mean}} )</th>
<th>( \epsilon_p^{\text{max}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_h = 1, N_n = 20 )</td>
<td>( 1.7 \times 10^{-6} )</td>
<td>0.0077</td>
<td>0.0368</td>
</tr>
<tr>
<td>( N_h = 1, N_n = 50 )</td>
<td>( 8.55 \times 10^{-7} )</td>
<td>0.0056</td>
<td>0.0289</td>
</tr>
<tr>
<td>( N_h = 2, N_n = 20 )</td>
<td>( 5.36 \times 10^{-7} )</td>
<td>0.0047</td>
<td>0.0176</td>
</tr>
<tr>
<td>( N_h = 2, N_n = 50 )</td>
<td>( 2.97 \times 10^{-7} )</td>
<td>0.0039</td>
<td>0.0206</td>
</tr>
<tr>
<td>( N_h = 2, N_n = 100 )</td>
<td>( 7.91 \times 10^{-7} )</td>
<td>0.0052</td>
<td>0.0315</td>
</tr>
</tbody>
</table>

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

Two-scale Cook’s membrane problem

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

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 \( C_{\text{mat}}^{\text{mat}} = D_{\text{mat}}^{\text{mat}} = 1 \)
- Fiber material \( C_{\text{fib}}^{\text{fib}} = D_{\text{fib}}^{\text{fib}} = 100 \)
- Surrogate model trained with 200 snapshots
- Relative error to compare microscopic stresses

\[
\epsilon_{P_{y,x}} := \frac{|P_{y,x}^{\text{FE2}} - P_{y,x}^{\text{ROM}}|}{\langle |P_{y,x}^{\text{FE2}}| \rangle}
\]

\( \langle |P_{y,x}^{\text{FE2}}| \rangle \): Averaged absolute stress

\[
W(F, \mu) = C_1 (\text{Tr}(F^T F) - 3) - 2 \ln (\det F)) + D_1 (\det F - 1)^2
\]
Numerical Examples

Two-scale Cook’s membrane problem

Macroscopic stress component $P_{yx}$

(a) $\text{FE}^2$

(b) $\text{FE with P-PODGPR}$

(c) Relative error

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

Two-scale Cook’s membrane problem

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

(a) FE$^2$  
(b) FE with P-PODGPQ  
(c) Relative error

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

Two-scale Cook’s membrane problem

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

(a) $\text{FE}^2$

(b) FE with P-PODGPGR

(c) Relative error
### Numerical Examples

Two-scale Cook's membrane problem

<table>
<thead>
<tr>
<th></th>
<th>$FE^2$</th>
<th>$FE$ with P-PODGPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Snapshot generation</td>
<td>-</td>
<td>60 min</td>
</tr>
<tr>
<td>POD + GPR</td>
<td>-</td>
<td>1 min</td>
</tr>
<tr>
<td>Online simulation</td>
<td>4800 min</td>
<td>1 min</td>
</tr>
</tbody>
</table>

$\Rightarrow$ 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


