Multi-Scale Modeling of Heterogeneous Elastic Solids based on Control of Modeling Errors in Local Quantities of Interest

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Outline

1. Goal-Oriented Adaptive Modeling (GOAM) Method of Heterogeneous Elastic Materials\textsuperscript{1,2}

2. Estimation of Local Modeling Error

3. Numerical Results

4. Concluding Remarks


1. GOAM Method

Example: Two-Phase Composite

1) Properties of matrix are deterministic
2) Properties of inclusions are random, governed by two random variables ($E$ and $\nu$) with truncated Gaussian probability distribution

3) Quantity of interest is:

\[ Q(u) = \int_{\Omega} \int_{D_Q} \varepsilon_{yy}(u) \, dx\,dP \]
1. GOAM Method

Initial Surrogate Model - Classical Homogenization

Exact (stochastic)

Surrogate (deterministic)

$E(x, \omega)$

Statistical averaging

Spatial averaging

(Homogenization)

$E_0$
1. GOAM Method

Homogenized strain field $\varepsilon_{yy}^0$

Mean Strain field $\varepsilon_{yy}$

Relative homogenization error $\frac{Q(u) - Q(u_0)}{Q(u)} = 73\%$
1. GOAM Method

Model Enhancement

<table>
<thead>
<tr>
<th>Relative error</th>
<th>Step 1</th>
<th>Step 2</th>
<th>Step 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>20%</td>
<td>15%</td>
<td>13%</td>
<td></td>
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</tbody>
</table>
1. GOAM Method

Assessment/Estimation of Modeling Error

- In terms of micro-mechanical features of the response or quantities of interest $Q(u)$.

- Residual-Based, i.e. if given the equivalent variational statement, or primal problem:

$$\int_{\Omega} E \nabla u \cdot \nabla v \, dx = \int_{\Omega} f \cdot v \, dx + \int_{\Gamma_t} t \cdot v \, ds \quad \forall v \in V \subset H^1(\Omega)$$

then introduce a dual problem for each $Q(u)$:

$$B(w, p) = Q(w), \quad \forall w \in V.$$
1. GOAM Method

Summary

<table>
<thead>
<tr>
<th>Primal Elastostatics Problem</th>
<th>$B(u, v) = F(v)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dual Problem</td>
<td>$B(v, p) = Q(v)$</td>
</tr>
</tbody>
</table>

Error Equation

If $\tilde{u}$ is any of the surrogate solutions of $u$, then the modeling error of $\tilde{u}$ in terms of the quantity of interest $Q(\cdot)$ is:

\[
Q(u) - Q(\tilde{u}) = B(u, p) - B(\tilde{u}, p)
\]

\[
= F(p) - B(\tilde{u}, p)
\]

Residual
1. GOAM Method

Drawbacks of the Error Assessment Process

- Computation of the dual problem is prohibitive if not impossible $\Rightarrow$ surrogate or homogenized solutions $p^0$ of $p$ are solved for instead to assess the error. Hence,

$$Q(u) - Q(\tilde{u}) \approx \frac{F(p^0) - B(\tilde{u}, p^0)}{\text{Error Estimate}}$$

However, estimate has often poor accuracy.

- The surrogate descriptions of the dual problems still require solution of global problems, for each quantity of interest.
1. GOAM Method

Proposed New Approach

• Develop a local dual problem which can be solved numerically at high accuracy without the need for any surrogate or homogenized descriptions for the dual problem.

• Focus on estimating homogenization errors. It indirectly provides estimates of multi-scale surrogate solutions $\tilde{u}$:

$$Q(u) - Q(\tilde{u}) = Q(u) - Q(u^0) + Q(u^0) - Q(\tilde{u})$$

estimated

computed
2. Local Estimation of Modeling Error

Local Elasticity Problem

\[-\nabla \cdot E \nabla u = f \text{ in } D_Q\]

\[E \nabla u \cdot n = t_u \text{ on } \partial D_Q\]

Local Variational Formulation

\[\int_{D_Q} E \nabla u \cdot \nabla v \, dx = \int_{D_Q} f \cdot v \, dx + \int_{\partial D_Q} t_u \cdot v \, ds, \quad \forall v \in H^1(D_Q)\]
2. Local Estimation of Modeling Error

Local Dual Problem

\[ B_{\text{loc}}(v, p) = Q(v), \quad \forall v \]

- Since the dual problem is defined on a small domain \( D_Q \), containing a limited amount of micro-mechanical information, \( p \) can be easily numerically computed with extremely high accuracy.

- This problem is well-posed in \( H^1(D_Q)/\mathbb{R} \)

\[ \Downarrow \]

Only for functionals \( Q(\cdot) \) of local gradients of the displacements (i.e. stresses and strains) a dual solution \( p \) exists.
2. Local Estimation of Modeling Error

Summary

<table>
<thead>
<tr>
<th>Local Elasticity Problem</th>
<th>$B_{\text{loc}}(u, v) = F_{\text{loc}}(v)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Local Dual Problem</td>
<td>$B_{\text{loc}}(v, p) = Q(v)$</td>
</tr>
</tbody>
</table>

Error Equation

$$Q(u) - Q(u^0) = B_{\text{loc}}(u, p) - B_{\text{loc}}(u^0, p)$$
$$= F_{\text{loc}}(p) - B_{\text{loc}}(u^0, p)$$
2. Local Estimation of Modeling Error

Problem/Issue

• Error equation is not computable due to the presence of the unknown traction $t_u$ in $F_{\text{loc}}(p)$:

$$F_{\text{loc}}(p) = \int_{D_Q} f \cdot p \, dx + \int_{\partial D_Q} t_u \cdot p \, ds$$

Solution

• Estimate $F_{\text{loc}}(p)$ by considering the local description of the homogenized primal problem.
2. Local Estimation of Modeling Error

Local Homogenized Problem

\[- \nabla \cdot E^0 \nabla u^0 = f \text{ in } D_Q \]
\[E^0 \nabla u^0 \cdot n = t_{u^0} \text{ on } \partial D_Q\]

Local Variational Formulation

\[\int_{D_Q} E^0 \nabla u^0 \cdot \nabla v \, dx = \int_{D_Q} f \cdot v \, dx + \int_{\partial D_Q} t_{u^0} \cdot v \, ds, \forall v \in H^1(D_Q)\]

\[B^0_{loc}(u^0, v) = F^0_{loc}(v)\]
2. Local Estimation of Modeling Error

**Homogenized Local Problem**

\[ B_{loc}^0(u^0, v) = F_{loc}^0(v), \ \forall v \]

\[ \downarrow v = 1 \]

\[ B_{loc}^0(u^0, 1) = F_{loc}^0(1) \]

\[ \downarrow \]

\[ 0 = \int_{D_Q} f \, dx + \int_{\partial D_Q} t_{u^0} \, ds \]

**Exact Local Problem**

\[ B_{loc}(u, v) = F_{loc}(v), \ \forall v \]

\[ \downarrow v = 1 \]

\[ B_{loc}(u, 1) = F_{loc}(1) \]

\[ \uparrow \]

\[ 0 = \int_{D_Q} f \, dx + \int_{\partial D_Q} t_u \, ds \]

\[ \downarrow \]

\[ \int_{\partial D_Q} t_u \, ds = \int_{\partial D_Q} t_{u^0} \, ds. \]
2. Local Estimation of Modeling Error

Homogenization Error Estimate

Since the average values of the tractions of the exact fine-scale solution $t_u$ and the homogenized solution $t_{u^0}$ over the edge of $D_Q$ are the same, $F_{\text{loc}}(\cdot)$ in the error equation is estimated by the homogenized $F^0_{\text{loc}}(\cdot)$:

$$Q(u) - Q(u^0) = F_{\text{loc}}(p) - B_{\text{loc}}(u^0, p)$$

$$\approx F^0_{\text{loc}}(p) - B_{\text{loc}}(u^0, p)$$  
Computable

$$= B^0_{\text{loc}}(u^0, p) - B_{\text{loc}}(u^0, p)$$  

$$\overset{\text{def}}{=} \int_{D_Q} (E^0 - E) \nabla u^0 \cdot \nabla p \, dx$$  

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2. Local Estimation of Modeling Error

(Final) Estimate of Multiscale Modeling Error

Let \( u \) be the exact solution, \( \tilde{u} \) a multiscale solution, and \( u^0 \) the homogenized solution, then:

\[
Q(u) - Q(\tilde{u}) = Q(u) - Q(u^0) + Q(u^0) - Q(\tilde{u})
\]

\[
\approx \int_{D_Q} (E^0 - E) \nabla u^0 \cdot \nabla p \, dx + Q(u^0) - Q(\tilde{u})
\]
2. Local Estimation of Modeling Error

\[ Q(u) - Q(\tilde{u}) \approx \int_{DQ} (E^0 - E) \nabla u^0 \cdot \nabla p \, dx + Q(u^0) - Q(\tilde{u}) \]

Local residual functional

Computing the estimate of the modeling error of a multiscale solution in terms of micro mechanical feature of interest \( Q(\cdot) \) requires:

- The first surrogate solution: the homogenized solution \( u^0 \).
- Solving for the dual solution \( p \) over a small region \( D_Q \) containing the micro mechanical feature of interest
- Computing a local residual functional over \( D_Q \) involving \( u^0 \) and \( p \).
3. Numerical Results

Two-Phase Composite Beam

1) $Q(u)$ is average strain $\varepsilon_{xx}$ in $\omega_i$, $i = 1, 2, 3, 4$

2) Material properties are deterministic
3. Numerical Example

Axial Strain Fields

Exact

Homog.
3. Numerical Example

Quantity of interest is average axial strain $\varepsilon_{xx}$ over each of the small subdomains $\omega_i, i = 1, \ldots, 4$. Thus,

$$ Q_i(u) = \frac{1}{|\omega_i|} \int_{\omega_i} \frac{\partial u_x}{\partial x} \, dx $$

Local Dual Problems

$$ B_{\text{loc}}(v, p_i) = Q_i(v), \quad \forall v $$

$$ \therefore $$

$$ \int_{\omega_i} E \nabla v \cdot \nabla p_i \, dx = \frac{1}{|\omega_i|} \int_{\omega_i} \frac{\partial v_x}{\partial x} \, dx, \quad \forall v $$
3. Numerical Example

Local Dual Solution in $\omega_1$

\[
\frac{\partial p_x}{\partial x}, \quad \frac{\partial p_y}{\partial y}
\]
3. Numerical Example

Local Domain of Interest

<table>
<thead>
<tr>
<th>Effectivity index</th>
<th>$\omega_1$</th>
<th>$\omega_2$</th>
<th>$\omega_3$</th>
<th>$\omega_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>estimator $= \frac{Q(u) - Q(u^0)}{Q(u) - Q(u^0)}$</td>
<td>1.04</td>
<td>1.09</td>
<td>1.34</td>
<td>1.14</td>
</tr>
</tbody>
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4. Concluding Remarks

- An estimator of modeling errors in local stresses and strains has been developed that involves solving a local dual problem and computing local residual integrals.

- The estimator exhibits high accuracy.

- Estimation of multiple local modeling errors is computationally feasible.
4. Concluding Remarks

- Estimator is currently extended to the analysis of stochastic and nonlinear problems.

- Since the dual problem is only well-posed if the quantity of interest involves gradients of the displacements, alternative local dual problems need to be investigated to broaden the applicability of the estimator.