Numerical Evaluation of Interaction Tensors in Heterogeneous Materials

Reduced Order Modeling for Composites

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• Multiscale modeling

• Transformation Field Analysis (TFA)
  – Theory
  – Offline and online stage

• Offline stage
  – Spatial decomposition of the RVE
  – Determination of interaction tensors

• First TFA results for UD fibers
Aim: achieving macroscopic material response $\bar{\varepsilon} \rightarrow \bar{\sigma}$

Linking microscopic and macroscopic scales: $x \leftrightarrow X$
- Model macroscopic behaviour by respecting microscopic processes
- Taking into account microscopic structure

Strategy: finding a representative volume element (RVE)

RVE represents the micro-structure at a macroscopic point
• Computing macroscopic response: solving boundary value problems for a RVE
  – FEM: solving equations for all microscopic points

→ computational effort is too high with the FEM

• Finding a less costly way to achieve macroscopic response?
  → Reduced Order Modeling (ROM) approaches
Subdivision of the full RVE volume $V$ into a number $r$ subvolumes $V_r$.

Piecewise uniform fields of internal variables in the clusters:

$$\alpha_r(x) = \alpha_r.$$

Local fields

$$\alpha(x) = \sum_{r=1}^{k} \chi_r \alpha_r,$$

where

$$\chi_r = \begin{cases} 1, & x \in V_r \\ 0, & \text{else} \end{cases}$$

Internal variables:

$$\alpha_r = \varepsilon_r, \varepsilon_r^{in}, \sigma_r, \sigma_r^{eig}.$$
• Overall stress and strain

\[ \overline{\sigma} = \sum_{r=1}^{k} \nu_r \sigma_r, \quad \overline{\varepsilon} = \sum_{r=1}^{k} \nu_r \varepsilon_r \]

• Local constitutive relation:

\[ \sigma_r = C_r : (\varepsilon_r - \varepsilon_r^{in}) \]

\[ \sigma_r^{eig} = -C_r : \varepsilon_r^{in} \]
Microscopic – macroscopic coupling constitutive relation

\[ \varepsilon_r = A_r : \bar{\varepsilon} + \sum_{s=1}^{k} D_{rs} : \varepsilon_{s}^{in} \]

Elasto-plasticity:

\[ A_r^{ep} = [I + D_{rs} : (C_s^{-1} : C_s^{tan} - I)]^{-1} : A_r \]

Solving equations for clusters instead of all microscopic points

Evaluation of strain concentration tensors \( A \) and interaction tensors \( D \)
• TFA: reduce computational cost for multiscale simulations by a spatial decomposition of the RVE

• Problem: capturing the highly heterogeneous strain and plastic strain field → Cluster decomposition based on strain concentration tensors

• Offline computations
  – Cluster Decomposition
  – Once-for-all computation: strain concentration tensors $\mathbb{A}_r$ and interaction tensors $\mathbb{D}_{rs}$

• Online stage
  – Solve TFA equation for the clusters instead for all material points

\[ \varepsilon_r = \mathbb{A}_r : \bar{\varepsilon} + \sum_{s=1}^{k} \mathbb{D}_{rs} : \varepsilon^\text{in}_s \]
TFA Overview

• Offline stage:

1) full FEM simulations

Extract strain concentration tensors $\mathbb{A}(x)$

2) Clustering of the RVE in $r$ clusters and determination of the $\mathbb{A}_r$

3) FEM simulations with eigenstrain to determine the $\mathbb{D}_{rs}$
Cluster Decomposition

- Clustering of all microscopic points based on similarity of mechanical behavior
  → Required: strain concentration tensors for all microscopic points

\[ \varepsilon(x) = \mathcal{A}(x) : \bar{\varepsilon} \]

- Determination of 36 independent components of \( \mathcal{A}(x) \):
  application of 6 orthogonal loading conditions \( \bar{\varepsilon} \) on the RVE

- Simulations in the elastic range
Cluster Decomposition

- UD fibers
- Results for various cluster numbers $k = 2, 4, 12$ for the matrix
Analytical evaluation including Green’s function
- Provides influences between material points at different locations
- Relies on homogenized material properties, isotropic or anisotropic

Composites: Microscopic strongly heterogeneous properties
→ Homogenized anisotropic stiffness not representative

Ability to account for complex anisotropic + heterogeneous structures

Numerical instead of analytical determination of eigenstrain – strain interaction tensors
• BC: periodic, no overall strain: $\bar{\varepsilon} = 0$

$$\varepsilon_r = A_r : \bar{\varepsilon} + \sum_{s=1}^{k} \mathbb{D}_{rs} : \varepsilon_s^{eig} \quad \Rightarrow \quad \varepsilon_r = \sum_{s=1}^{k} \mathbb{D}_{rs} : \varepsilon_s^{eig}$$

• 3D: Application of 6 orthogonal eigenstrains in cluster $s$ and computation of resulting strain in cluster $r$ to determine 36 independent components of $\mathbb{D}_{rs}$
Interaction Tensors

- Dilatation of clusters with eigenstrain
- Compression of surroundings

$k = 4$

Cluster distribution

\[ \varepsilon_{yy} \]
\[ \varepsilon_{xx} \]
\[ \varepsilon_{yy} \]
• Results comparison: FEM vs. TFA

TFA Results

\[ \varepsilon \] [MPa]

17 clusters

3 clusters

\[ t=0.02 \]
Conclusions

- Elasticity: good accuracy
- Plastic deformation starts later
- Highly over-stiff behavior when elastic range is exceeded
- Bad representation of highly localized plastic strain

- Increase number of clusters → increasing computational effort
- Switch to NTFA → extensive pre-simulations and savings required
References

• Transformation Field Analysis:


  Pierre Suquet (1997), Continuum Micromechanics, Springer

• Non-uniform Transformation Field Analysis: