Goal-oriented adaptivity based on a model hierarchy of mean-field and full-field homogenization methods in linear elasticity

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Summary
Homogenization methods are drawing increasing attention for simulation of heterogeneous materials like composites. For balancing the accuracy and the numerical efficiency of such strategies, we deal with both model and discretization errors of the finite element method (FEM) on a macroscale. Within a framework of goal-oriented adaptivity, we consider linear elastic heterogeneous materials, for which first-order homogenization schemes apply. A novel model hierarchy is proposed based on mean-field and full-field homogenization methods. For the former, we consider several well-established schemes like Mori-Tanaka or self-consistent as basic models, and for the latter, as superior models, unit cell problems are solved via the FEM under an a priori chosen boundary condition. For a further stage of the model hierarchy, we consider hierarchical unit cells within the frame of the FEM toward an adaptive selection of the unit cell size. By means of several numerical examples, we illustrate the effectiveness of the proposed adaptive approach.

KEYWORDS
adaptive finite element method, full-field methods, goal-oriented error estimate, mean-field methods, model adaptivity, unit cell size

1 | INTRODUCTION

Many engineering materials like steel, alloy, and composites are heterogeneous, when viewed on a certain (for instance micro) scale. On that scale, several constituents of different material properties can be distinguished. Under the premise that the individual material properties as well as the distribution of the different constituents are known, homogenization methods provide a powerful tool to predict their overall behavior, which is often of engineering interest. Another advantage of homogenization methods is their potential on optimum material design by avoiding high experimental cost. For a comprehensive overview, the interested reader is referred to related works. In this work, we limit our attention to methods assuming a clear scale separation, that is, the characteristic length of the subscale is much smaller than that of the macroscale. More specifically, we focus on the following classes of homogenization methods.

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Mean-field methods: They are established on the basis of the Eshelby solution to an ellipsoidal inclusion embedded in an infinite matrix, see, eg, Mori-Tanaka, self-consistent, and interaction direct derivative (IDD), and also find applications to nonlinear materials, see, eg, related works. By means of analytical solutions, this kind of methods is most efficient. As a drawback, they are not able to account for complex microstructures and some further effects like unit cell size or periodic boundary conditions. As an important feature, they resolve the microscopic fields only to their means over the individual material phases.

Full-field methods: They achieve a much higher resolution of the microscopic fields than the mean-field methods. A most straightforward way is to adopt computational methods at the expense of a large computational cost, see, eg, the works of Zohdi and Wriggers and Feyel and Chaboche for the FE method and the works of Moulinec and Suquet and Michel et al for fast fourier transformation–based methods.

Clearly, there are many other classes of homogenization methods like model-order reduction methods, higher-order homogenization schemes in nonlocal continua, variational methods, asymptotic homogenization, and distribution-enhanced homogenization framework (DEHF) considering higher-order moments, etc. Depending on what microscopic resolution they achieve, they also may fall into one of the aforementioned two categories. For other classifications covering a broad variety of homogenization methods, we refer to the recent review articles.

Furthermore, the influence of different microboundary conditions on the effective properties are examined, eg, in related works. The Dirichlet-type and the Neumann-type boundary condition are shown to provide the upper and the lower bounds, respectively. The periodic boundary condition usually shows the fastest convergence behavior, when the size of the chosen unit cell is enlarged. In this context, we refer to a unit cell as an arbitrary sample of microstructure, which does not necessarily meet the requirements of a representative volume element (RVE) according to Hill.

An RVE is entirely typical of the whole mixture on average. An RVE contains a sufficient number of inclusions for the apparent effective properties to be independent of the surface values of traction and displacement.

The apparent effective properties refer to those provided by a unit cell. For a unit cell to be an RVE, its size should be sufficiently large. The issue of a minimum RVE size is addressed, eg, in the work of Drugan and Willis. To address the issue of numerical model validation, the notion of model adaptivity has been well established for both linear and nonlinear problems. It aims at an adaptive model selection to efficiently achieve a preset level of accuracy, for which an assessment of model error is required. In this context, a model hierarchy, consisting of a series of mathematical models, from the simplest to the most complex (state-of-the-art) model with an ascending hierarchical order, plays a central role. A model, which is of a higher hierarchical order than the current one, can be used for both error estimate and a possible model refinement. If the error estimate is directed to a user-defined quantity of interest, the resulted adaptivity is called goal-oriented adaptivity, see, eg, other works. For applications to multiscale problems, we refer to related works. The issue of numerical verification is addressed by the adaptive FEM, which is developed to estimate and adaptively control the discretization error, see, eg, other works for the general framework of a posteriori error estimate and some related works for goal-oriented error estimate.

In our recent work, a general coupled framework of model adaptivity and adaptive FEM was developed for linear elastic heterogeneous materials. For a model hierarchy, a bounding theory according to Dederichs and Zeller and Kröner was used.

In this paper, as novelties compared to existing literature, we pursue the following goals.

- We propose a novel model hierarchy for model adaptivity based on mean-field and full-field homogenization methods.
- For theoretical consistency of the model hierarchy, the mean-field and the full-field methods are interpreted as different approximations of full-field formulations.
- Full-field methods are only applied on those regions where mean-field methods are not sufficiently accurate. In this manner, benefits of both methods, ie, accuracy of full-field methods and numerical efficiency of mean-field methods, can be fully exploited.
- Within the frame of full-field methods, adaptive selection of unit cell size is done for an enhanced numerical efficiency.
- For a fast convergence behavior with respect to the unit cell size, an appropriate boundary condition is determined prior to the computation. To this end, different microboundary conditions are examined.
- The aforementioned model aspects of mean-field and full-field methods, unit cell size, and microboundary conditions are integrated into a single model hierarchy.
- The resulting adaptive algorithm on model adaptivity is coupled to mesh adaptivity for balancing related error sources, ie, model and discretization errors on the macroscale. It is driven by goal-oriented error estimates for error control w.r.t. a quantity of interest.
This paper is structured as follows. In Section 2, the general framework of a two-scale modeling is introduced, including the aspects of scale separation, scale transition, and related boundary conditions as well as a full-field formulation toward effective properties. An equivalent mean-field formulation to the full-field formulation is established at the beginning of Section 2.3. Subsequently, several well-established mean-field and FE-based full-field methods are revisited and interpreted as two different approximations of full-field formulations. Section 3 briefly reviews the coupled adaptive strategy developed in our previous work for a structural analysis. Subsequently, a novel model hierarchy is proposed and discussed in some detail. Several numerical experiments are presented in Section 4, whereas Section 5 gives a conclusion and an outlook on further research.

Notation. The scalar products of two vectors \( \mathbf{a} \) and \( \mathbf{b} \) and two second-order tensors \( \mathbf{A} \) and \( \mathbf{B} \) are

\[
\mathbf{a} \cdot \mathbf{b} = a_i b_i, \quad \mathbf{A} : \mathbf{B} = A_{ij} B_{ij},
\]

respectively, using the Einstein summation convention for repeated indices. The gradient operator \( \nabla \) is introduced as

\[
\nabla \mathbf{c} := \mathbf{c} \otimes \nabla = c_{ij} \mathbf{e}_i \otimes \mathbf{e}_j \quad \text{with} \quad c_{ij} = \frac{\partial c_i}{\partial X_j},
\]

where \( \mathbf{e}_i, i = 1, 2, 3 \) is a Cartesian orthonormal basis and \( X_i \) are coordinates of the reference position \( X \). The divergence operator \( \text{Div}(\bullet) \) is defined as

\[
\text{Div}(\sigma) := \sigma \cdot \nabla = \sigma_{ij,j} e_i \quad \text{with} \quad \sigma_{ij,j} = \frac{\partial \sigma_{ij}}{\partial X_j}.
\]

Additionally, the volume averaging operator on a domain \( \Omega \) is defined as

\[
\langle \bullet \rangle = \frac{1}{|\Omega|} \int_{\Omega} \bullet \, dv.
\]

Gâteaux differentiation of a linear form \( F \) and a bilinear form \( B \) w.r.t. the argument \( u \) is denoted as

\[
\begin{align*}
\mathcal{D}_u F(u; v) &= \lim_{\theta \to 0} \frac{1}{\theta} [F(u + \theta v) - F(u)], \\
\mathcal{D}_u B(u; w, v) &= \lim_{\theta \to 0} \frac{1}{\theta} [B(u + \theta v; w) - B(u; w)],
\end{align*}
\]

respectively.

2 A TWO-SCALE PROBLEM AND ITS SURROGATE MODELS

2.1 Scale separation and transition

By means of the asymptotic homogenization theory, we consider a two-scale mechanical problem of first order, making the assumption of scale separation, i.e., \( l/L \ll 1 \), as depicted in Figure 1. To each material point of the macrodomain \( \Omega \), a microdomain \( \Omega \), i.e., the RVE, is associated, where subscripts 0 and \( t \) denote the reference and the current configuration, respectively.

![Illustration of a two-scale problem](image-url)
Neglecting the difference between the reference and the current configuration, we assume a framework of small strains, with the macrodisplacement vector and the macrosmall strain tensor as

\[ \mathbf{u} = \mathbf{x} - \mathbf{X}, \]  

\[ \epsilon = \nabla_{\text{sym}} \mathbf{u}, \]  

respectively. In Equation (6a), \( \mathbf{X} \) and \( \mathbf{x} \) are the position vectors with respect to a reference point \( O \), respectively, in the reference and the current state. Moreover, the macroscopic equilibrium problem \( \overline{P} \) and the underlying microscopic equilibrium problem \( P \) read

\[ \overline{P} : \begin{cases} \text{Div} (\overline{\sigma}) + \overline{b} = 0, & \text{in } \Omega \\ \overline{\sigma} \mathbf{N} = \overline{i}, & \text{on } \Gamma_i \\ \overline{\mathbf{u}} = \overline{\mathbf{u}}^*, & \text{on } \Gamma_u, \end{cases} \]  

\[ P : \begin{cases} \text{Div} (\sigma) = 0, & \text{in } \Omega \\ + \text{ boundary conditions}, \end{cases} \]

respectively. In problem \( \overline{P} \), \( \overline{\sigma} \) denotes the macroscopic stress tensor and \( \overline{i} \) represents the tractions imposed on \( \Gamma_i \) satisfying the Neumann boundary condition. The body force is symbolized by \( \overline{b} \), whereas \( \overline{\mathbf{u}}^* \) indicates the prescribed displacements on the Dirichlet boundary \( \Gamma_u \) with the properties \( \Gamma_u \bigcup \bigcap \Gamma_i = \overline{\Gamma} \) and \( \Gamma_u \bigcap \bigcap \Gamma_i = \emptyset \), where \( \overline{\Gamma} \) symbolizes the total boundary for the macroscopic problem. To solve the macroproblem \( \overline{P} \) with the FEM, let us establish its weak form

\[ \int_{\Omega} \overline{\epsilon} : \overline{\delta \mathbf{u}} = \int_{\Omega} \overline{\delta \mathbf{u}} \cdot \overline{b} dV + \int_{\Gamma_i} \overline{\delta \mathbf{u}} \cdot \overline{i} dA, \quad \forall \overline{\delta \mathbf{u}} \in \overline{V}, \]  

where \( \overline{\mathbf{u}} \) and \( \delta \overline{\mathbf{u}} \) are the macrodisplacement vector and its variation, respectively. \( \overline{V} \) is an appropriate Sobolev space. For linear elasticity, \( \overline{B}(\cdot ; \cdot) \) is a bilinear form, whereas \( \overline{F} (\cdot ) \) is a linear form. We shall rewrite Equation (8) in a residual form as

\[ \phi (\overline{\mathbf{u}}; \delta \overline{\mathbf{u}}) := \overline{F}(\delta \overline{\mathbf{u}}) - \overline{B}(\overline{\mathbf{u}}, \delta \overline{\mathbf{u}}) = 0. \]  

Microproblem \( P \) is completed with some proper boundary conditions. This will be separately discussed in Appendix A.1. Moreover, \( \sigma \) and \( \epsilon \) are, respectively, the microscopic stress and the microscopic strain tensor, which are generally heterogeneously distributed within the RVE, whereas \( \overline{\epsilon} \) denotes the macroscopic strain tensor.

Additionally, the scale transition, which couples both problems \( \overline{P} \) and \( P \), is established by

\[ \overline{\epsilon} = \langle \epsilon (x) \rangle, \]  

\[ \overline{\sigma} = \langle \sigma (x) \rangle, \]  

\[ \langle \sigma ; \epsilon \rangle = \langle \sigma \rangle ; \langle \epsilon \rangle = \overline{\sigma} : \overline{\epsilon}, \]  

where Equation (10c) is nothing else but the well-established Hill-Mandel condition.\(^{36}\) Being consistent with the Hill-Mandel condition (10c), we consider three different boundary conditions described in Appendix A.1.

### 2.2 Localization operators and effective properties

**Full-field formulations:** For linear elastic materials, the following two equivalent linear constitutive relations apply:

\[ \sigma (x) = \mathbb{C} (x) \epsilon (x), \]  

\[ \epsilon (x) = \mathbb{S} (x) \sigma (x), \]

with the microelasticity tensor \( \mathbb{C} \) and the microcompliance tensor \( \mathbb{S} = \mathbb{C}^{-1} \), respectively. A common approach toward a structural (macroscopic) analysis consists of two steps, ie, (1) solve the microproblem (7b) and (2) perform the scale
transition (10a) or (10b). For the first step, the microproblem (7b) can be defined either via a prescribed macrostrain $\xi$ or via a prescribed macrostress $\sigma$. Accordingly, there exist linear localization operations

$$
\varepsilon(x) = A(x) \xi, \quad (12a)
$$

$$
\sigma(x) = B(x) \sigma, \quad (12b)
$$

where $A$ and $B$ are referred to as the microstrain and the microstress localization tensor, respectively. Moreover, inserting Equation (12a) into Equation (10a) renders the identity

$$
\langle A(x) \rangle = I_S, \quad (13)
$$

where $I_S$ denotes the fourth-order symmetric identity tensor. Similarly, by inserting Equation (12b) into Equation (10b), we obtain

$$
\langle B(x) \rangle = I_S. \quad (14)
$$

Equations (12a) and (12b) can be interpreted as formal solutions of the microproblem (7b).

For the second step, we combine Equations (12a), (11a), and (10b) and obtain

$$
\sigma = \langle C(x) A(x) \rangle \xi, \quad (15)
$$

for a prescribed $\xi$, where we refer to $C$ as the effective elasticity tensor. If $\sigma$ is prescribed, one may use Equation (12b) in combination with Equations (11b) and (10a) and obtain

$$
\xi = \langle S(x) B(x) \rangle \sigma, \quad (16)
$$

where $S$ is nothing else but the effective compliance tensor.

**Mean-field formulations:** In contrast to the full-field representations (11a)-(16), the mean-field methods resolve the relevant microscopic fields to their means over $N$ individual material phases distinguished by a subscript $r = 0, 1, \ldots, N-1$. Correspondingly, the localization rules (12a) and (12b) reduce to

$$
\varepsilon_r = A_r \xi, \quad (17a)
$$

$$
\sigma_r = B_r \sigma, \quad (17b)
$$

where $A_r$ and $B_r$ are the average strain and the average stress localization tensor, respectively, and

$$
\varepsilon_r = \langle \varepsilon \rangle_{\Omega_r}, \quad (18a)
$$

$$
\sigma_r = \langle \sigma \rangle_{\Omega_r}, \quad (18b)
$$

are the average strain and the average stress tensor over the local domain $\Omega_r$ occupied by the $r$th material phase, respectively. By inserting Equations (12a) and (17a) into Equation (18a) and inserting Equations (12b) and (17b) into Equation (18b), we obtain

$$
A_r = \langle A \rangle_{\Omega_r}, \quad (19a)
$$

$$
B_r = \langle B \rangle_{\Omega_r}, \quad (19b)
$$

respectively. The mean-field version of effective properties are obtained from Equations (15) and (16) as

$$
C = \sum_{r=0}^{N-1} c_r C_r A_r, \quad (20a)
$$
respectively. Here, $c_r$, $C_r$, and $S_r$ represent the volume fraction, the elasticity tensor, and the compliance tensor of the phase $r$, respectively. Correspondingly, Equations (13) and (14) become

$$
\sum_{r=0}^{N-1} c_r A_r = \mathbb{I},
$$

(21a)

$$
\sum_{r=0}^{N-1} c_r B_r = \mathbb{I},
$$

(21b)

respectively. The aforementioned mean-field formulations are equivalent to the full-field ones (11a)-(16) in the sense of determining effective properties. Up to now, no approximations have been made.

### 2.3 Approximations of full-field formulations

The exact solution of the microproblem (7b), formally in Equation (12a) or Equation (12b), is generally intractable. In the following, we first show that the full-field formulation in Section 2.2 may equivalently reduce to a mean-field formulation, which forms a basis for the mean-field methods. Subsequently, well-established mean-field and full-field methods are revisited and interpreted as two different approximations of full-field formulations. As a full-field method, we adopt the FEM to achieve a full-field approximation.

#### 2.3.1 Mean-field approximations

The mean-field methods are fundamental in micromechanics. In this section, we review some well-established mean-field methods based on the mean-field formulation in Section 2.2. It is obvious from Equations (22a) and (22b) that the effective properties $C$ or $S$ require the knowledge about the localization tensors $A_i$ or $B_i$ of each single inclusion $i = 1, \ldots, N_i$. These localization tensors are determined by means of a single inclusion problem illustrated in Figure 2B.

In this work, we consider some composite materials of matrix-inclusion type, as shown in Figure 2A. For our convenience, subscript 0 is assigned to the matrix material, whereas the subscript $i = 1, \ldots, N_i$ denotes the $i$th inclusion. Consequently, we have $r = [0, i]$ and $N_i = N - 1$. In combination with Equations (21a) and (21b), Equations (20a) and (20b) become

$$
\overline{C} = C_0 + \sum_{i=1}^{N_i} c_i (C_i - C_0) A_i,
$$

(22a)

$$
\overline{S} = S_0 + \sum_{i=1}^{N_i} c_i (S_i - S_0) B_i,
$$

(22b)

respectively.

**Eshelby’s solution:** The origin of the mean-field approximate methods may be traced back to the seminal work of Eshelby, who considered an infinite matrix material with an ellipsoidal inclusion $i$, which is made of the same material with the property $C'$ but with a uniform eigenstrain $\varepsilon_i^s$, see Figure 2C. No remote load is applied. The strain field in that inclusion induced by the release of $\varepsilon_i^s$ is uniform and can be expressed as

$$
\varepsilon_i^e = S_i^e \varepsilon_i^s,
$$

(23)
where \( S'_i \) is the Eshelby tensor depending on the material property \( C' \) as well as the shape and orientation of inclusion \( i \). Additionally, superscript \( e \) stands for this eigenstrain problem. The corresponding stress is obtained from

\[
\sigma^e_i = C' (\varepsilon^e_i - \varepsilon^+_i) = C' (S'_i \varepsilon^+_i - \varepsilon^+_i) = -C'_i \varepsilon^+_i,
\]

where the eigenstiffness tensor is defined as

\[
C'_i := C' (\mathbb{S} - S'_i).
\]

**The equivalent inclusion concept:** For the actual composite material in Figure 2A with \( N_i \) inclusions, the localization tensors \( A_i \) in Equation (22a) or \( B_i \) in Equation (22b) are determined by \( N_i \) single inclusion problems in Figure 2B. The interaction between different inclusions may be considered by modifying the matrix material properties \( C' \) or the remote load \( \varepsilon' \) or \( \sigma' \), see the Appendices B.2 to B.4. As shown in Figure 2B, inclusion \( i \) is made of a material with \( C_i \) other than \( C' \) of the matrix material, where we do not assume an eigenstrain. For the Eshelby’s solution of the problem in Figure 2C to apply, we may find a proper eigenstrain \( \varepsilon^+_i \) for a prescribed strain \( \varepsilon' \), such that the stresses in the inclusion of both cases are equivalent, ie,

\[
\sigma^e_i = C' (\varepsilon^e_i + \varepsilon^+_i) = C_i (\varepsilon' + \varepsilon^+_i),
\]

which, in combination with Equation (23), suggests the claimed eigenstrain

\[
\varepsilon^+_i = \left( (C_i - C') S'_i + C' \right)^{-1} \left( C' - C_i \right) \varepsilon',
\]

where we have split the strain within inclusion \( i \) into a constant and a fluctuation part, ie, \( \varepsilon_i = \varepsilon' + \varepsilon^e_i \). Together with Equations (23) and (27), we have

\[
\varepsilon_i = \varepsilon' + \varepsilon^+_i = \varepsilon' + S'_i \varepsilon^+_i = A'_i \varepsilon',
\]

where we identify

\[
A'_i = \left( \mathbb{S} + S'_i C'^{-1} (C_i - C') \right)^{-1}.
\]

Correspondingly, the stress in the inclusion \( i \) reads

\[
\sigma_i = C_i A'_i \varepsilon' = C_i A'_i S' \sigma' = B'_i \sigma',
\]

where we identify

\[
B'_i = C_i A'_i S' = (S_i - S_i (S_i - S'))^{-1} S'.
\]

In Appendix B, we consider some well-established mean-field methods by specifying the single inclusion problem in Figure 2B. The methods include approximations and simplifications. For instance, the subdivision of the actual composite problem into \( N_i \) single inclusion problems in Figure 2B is an approximation, which, together with the dilute method in Appendix B.1, completely neglects the inclusion interaction. The inclusion interaction can be considered to a certain extent, but not exactly, by some advanced schemes (Mori-Tanaka, self-consistent, and IDD) in the Appendices B.2 to B.4. Additionally, the mean-field methods in the Appendices B.1 to B.3 do not account for possible anisotropic inclusion distributions, whereas the IDD method in Appendix B.4 is restricted to ellipsoidal distributions. Hence, in contrast to the mean-field formulation in Section 2.2, the effective properties determined by the mean-field methods are not equivalent to those of the full-field formulation in Section 2.2, but approximations.

### 2.3.2 FE approximations

Now, we consider the FEM as a further approximation of the microproblem (7b). Next, we introduce a weak residual form of the microproblem (7b)

\[
\varphi (u; \delta u) = \int_\Gamma \delta u \cdot t dA - \int_{\Omega} \varepsilon \left[ \delta u \right] : \sigma \left[ u \right] dV = 0, \quad \forall \delta u \in V^0,
\]

(32)
where \( B, F, \) and \( \mathcal{V}^0 \) are a bilinear form, a linear form, and an appropriate Sobolev space, respectively. Clearly, the primal solution of (32) is the microdisplacement vector \( \mathbf{u} \). By introducing a regular FE-space \( \mathcal{V}^0_h \), we may further arrive at a discretized version of (32)

\[
\varphi(\mathbf{u}_h; \delta \mathbf{u}_h) = F(\delta \mathbf{u}_h) - B(\mathbf{u}_h; \delta \mathbf{u}_h) = 0, \quad \forall \delta \mathbf{u}_h \in \mathcal{V}^0_h.
\]

(33)

The implementation of different boundary conditions is outlined in Appendix A.2. Due to the heterogeneous microscopic fields considered by the FEM, we shall refer the FE approximations to as full-field methods.

### 2.3.3 Comparative adjustment

As discussed in the Sections 2.3.1 and 2.3.2, mean-field and full-field methods are surrogate models of the exact full-field formulations (11a)-(16). Figure 3A schematically depicts the relation between solution spaces of mean-field and FE approximations as well as an exact solution. For illustration purposes, material properties (such as elasticity, plasticity or damage) and microstructural information (like inclusion shape or distribution) are chosen as independent variables. Note that inelasticity will not be considered in this work for simplicity. In particular, we assume that the solution space of the mean-field approximation is completely included within that of the FE approximation. Since the FEM allows to consider some fine micromorphology effects, which cannot be considered analytically via a mean-field approximation, it is expected to be more accurate than the mean-field methods in general. However, the FE approximation is still not exact due to the underlying discretization errors or due to the lack of knowledge about an RVE.

### 3 GOAL-ORIENTED ADAPTIVITY ON THE MACROSCALE

With the different approximation methods for homogenization introduced in the previous Sections 2.3.1 and 2.3.2 at hand, we are now in a position to establish the macroscale adaptivity. To this end, we first briefly recall the general goal-oriented adaptive approach developed in our previous work. Then, we propose a novel model hierarchy, including the aspects of mean-field and full-field homogenization methods as well as unit cell size.

#### 3.1 Quantity of interest and dual problem

For the exact model (9) to be practically solved, we need to introduce two additional models: the working (surrogate) model

\[
\varphi^{(n)}(\mathbf{u}_h^{(n)}; \delta \mathbf{u}_h) = F(\delta \mathbf{u}_h) - B^{(n)}(\mathbf{u}_h^{(n)}; \delta \mathbf{u}_h) = 0, \quad \forall \delta \mathbf{u}_h \in \mathcal{V}^0_h.
\]

(34)

with a hierarchical order \( n \geq 0 \) and the computable model

\[
\varphi^{(n)}(\mathbf{u}_h^{(n)}; \delta \mathbf{u}_h) = F(\delta \mathbf{u}_h) - B^{(n)}(\mathbf{u}_h^{(n)}; \delta \mathbf{u}_h) = 0, \quad \forall \delta \mathbf{u}_h \in \mathcal{V}^0_h.
\]

(35)

Here, \( \mathcal{V}^0_h \subset \mathcal{V}^0 \) represents the approximate FE-space. In the case where the quality of the simulation is measured by a quantity of interest \( Q(\mathbf{u}) \) depending on a macroscale solution \( \mathbf{u} \), we define the total error \( E \) as

\[
E(\mathbf{u}, \mathbf{u}_h^{(n)}) := Q(\mathbf{u}) - Q(\mathbf{u}_h^{(n)}).
\]

(36)
For duality techniques\textsuperscript{46,47,53} to apply, we first formulate a residual as
\[
\tilde{\sigma} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) = \mathbf{F} \left( \delta \mathbf{u} \right) - \mathbf{B} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) = \mathbf{B} \left( \mathbf{u}; \delta \mathbf{u} \right) - \mathbf{B} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) = \mathbf{B} \left( \mathbf{e}; \delta \mathbf{u} \right),
\]  
(37)

with the error of the primal solution \( \mathbf{e} = \mathbf{u} - \mathbf{u}_h^{(n)} \), where we used the Galerkin orthogonality (9) for the second equality and the last equality is ensured by the fact that \( \mathbf{B} \) is bilinear. Since the quantity of interest \( Q \) in Equation (36) does not necessarily have to be linear, we rewrite Equation (36) as
\[
E \left( \mathbf{u}, \mathbf{u}_h^{(n)} \right) = Q \left( \mathbf{u} \right) - Q \left( \mathbf{u}_h^{(n)} \right) = Q_S \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \mathbf{e} \right),
\]
(38)
where we introduce a secant form as
\[
Q_S \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \mathbf{e} \right) = \int_0^1 \mathbf{D}_\mathbf{\omega} Q \left( \mathbf{u}_h^{(n)} + s \mathbf{e}; \mathbf{e} \right) ds,
\]
(39)
with \( 0 \leq s \leq 1 \) (see also the work of Rüter\textsuperscript{56}).

To set a link between Equations (37) and (39), we introduce a dual Lagrangian functional \( \mathcal{L} \) as
\[
\mathcal{L} \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \mathbf{z}; \delta \mathbf{z} \right) := Q_S \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \delta \mathbf{z} \right) - \mathbf{B}^* \left( \mathbf{z}, \delta \mathbf{z} \right),
\]
(40)
where \( \mathbf{B}^* \) is the adjoint form of \( \mathbf{B} \), satisfying \( \mathbf{B}^* \left( \mathbf{z}, \delta \mathbf{z} \right) = \mathbf{B} \left( \mathbf{z}; \delta \mathbf{z} \right) \). Furthermore, \( \delta \mathbf{z} \in \mathbf{V}_h^0 \) and \( \mathbf{z} \in \mathbf{V}_h^0 \) are test functions. The dual problem is then established by
\[
\text{stat}_{\delta \mathbf{z}} \left\{ \mathcal{L} \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \mathbf{z}; \delta \mathbf{z} \right) \right\} \quad \Rightarrow \quad Q_S \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) - \mathbf{B} \left( \mathbf{z}, \delta \mathbf{u} \right) = 0,
\]
(41)
with the dual solution \( \mathbf{z} \). For self-adjoint problems (true for the present case), we have
\[
\mathbf{B} \left( \mathbf{z}, \delta \mathbf{u} \right) = Q_S \left( \mathbf{u}, \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right).
\]
(42)

### 3.2 Exact error representations

To distinguish two different error sources, we rewrite the residual (37) as
\[
\tilde{\sigma} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) = \mathbf{F} \left( \delta \mathbf{u} \right) - \mathbf{B} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) = \mathbf{F} \left( \delta \mathbf{u} \right) - \mathbf{B} \left( \delta \mathbf{u}_h^{(n)} \right) + \mathbf{B} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) - \mathbf{B} \left( \mathbf{u}_h^{(n)}; \delta \mathbf{u} \right) := \tilde{\sigma}_h
\]
\[
:= \bar{\sigma}_m
\]
(43)

which defines the discretization error \( \tilde{\sigma}_h \) and the model error \( \tilde{\sigma}_m \) (see also the works of Larsson and Runesson\textsuperscript{47,53}). Note that the special cases \( \tilde{\sigma} = \tilde{\sigma}_m \) and \( \tilde{\sigma} = \tilde{\sigma}_h \) are obtained for \( h \to 0 \) and \( n \to \infty \), respectively. Finally, by combining Equations (36), (37), (38), (42), and (43), we obtain
\[
E \left( \mathbf{u}, \mathbf{u}_h^{(n)} \right) = \tilde{\sigma}_h \left( \mathbf{u}_h^{(n)}; \mathbf{z} - \pi \mathbf{z} \right) + \tilde{\sigma}_m \left( \mathbf{u}_h^{(n)}; \mathbf{z} \right).
\]
(44)

where \( E_h \) and \( E_m \) are the discretization error and the model error of the quantity of interest \( Q \), respectively. In Equation (44) for \( E_h \), the Galerkin orthogonality (35) is used, and \( \pi \mathbf{z} \in \mathbf{V}_h^0 \) is a projection of \( \mathbf{z} \) onto the FE-space \( \mathbf{V}_h^0 \).
3.3 A model hierarchy based on mean-field and full-field homogenization methods

To obtain a computable error estimate, some approximations are made in Appendix C. Next, we specify the exact, the working, and the fine model as

\[
B(u; \delta u) = \int_{\Omega} \varepsilon [\delta u] : (C \varepsilon [u]) \, dv, \tag{45a}
\]

\[
B^{(n)}(u; \delta u) = \int_{\Omega} \varepsilon [\delta u] : (C^{(n)} \varepsilon [u]) \, dv, \tag{45b}
\]

\[
B^{(n^+)}(u; \delta u) = \int_{\Omega} \varepsilon [\delta u] : (C^{(n^+)} \varepsilon [u]) \, dv, \tag{45c}
\]

respectively. Here, we choose \( n^+ = n + 1 > n \) for the fine model (45c).

In our previous work, a bounding theory according to Dederichs and Zeller and Kröner was used to establish a model hierarchy, i.e., to complete the working model (45b). In this work, we intend to combine different homogenization methods in Section 2.3. In doing so, we recall the solution spaces of mean-field and FE approximation in Figure 3A. On this basis, we propose a model hierarchy consisting of the following stages.

1. The basic model of hierarchical order \( n = 0 \) is chosen as one of the mean-field methods presented in Appendix B.
2. As an accuracy improvement, a further mean-field method is chosen as \( n = 1 \). Due to the lack of a hierarchical model structure, this method does not have to be computationally more expensive than the basic one. Most importantly, this choice eliminates the need of a full-field method for an error estimate of the basic model for \( n = 0 \). For a structural analysis, it is expected that the use of the two mean-field methods \( n = 0 \) and \( n = 1 \) is sufficient for a comparably large domain of the whole structure, and for both purposes of modeling and the error estimate to be specified in Equations (47), (48), and (49).
3. For a further accuracy improvement, the FE-based method in Equation (33) with an appropriately chosen boundary condition is adopted for \( n > 1 \) toward a full-field approximation. Here, the key role is played by hierarchical unit cells with increasing sizes \( n = n_s + 1 = 2, 3, \ldots \), see below for a more detailed discussion.

The aforementioned model hierarchy is based on the following assumptions.

- The hierarchy is formulated on an empirical basis, taking into account the performance of the different methods reported in the literature. As a result, the model hierarchy is actually not unique, and a specific choice is left to the user depending on the problem under study.
- It is assumed that the full-field homogenization method is always more accurate than any choice of mean-field strategy. For the chosen hierarchy, this means that the hierarchical level \( n = 2 \) gives a more accurate macrostress than level \( n_s = 0 \).
- No subscale FE-discretization errors are considered. With this, there is no a priori guarantee that the computational homogenization result (in terms of macroscale stresses) is more accurate than that obtained using the mean-field solution. In this work, FE-discretization errors of the full-field methods are assumed to be sufficiently small.

It is remarkable that the aspects of mean-field and full-field methods as well as hierarchical unit cells can be consistently included in one single-model hierarchy, as shown above. As a representative example, a model hierarchy used in Section 4 is as follows:

1. \( n = 0 \) : Self-consistent in Equation (B.12),
2. \( n = 1 \) : IDD in Equation (B.14),
3. \( n = n_s + 1 = 2, 3, \ldots \) : FEM (periodic) in Equation (A.7).

Based on the solution spaces of mean-field and FE approximations in Figure 3A, the resulting hierarchical models are schematically illustrated in Figure 3B.

An adaptive selection of microboundary conditions is not included in the model hierarchy, and a selection is suggested to be done prior to the adaptive approach, since, for our case, a switch of boundary conditions does not have a significant influence on the numerical effort associated with the FEM.

In the following, we give a respective discussion on the aspects of accuracy assessment and unit cell size.
TABLE 1 Comparative properties of several mean-field methods

| Methods                  | Accuracy  |
|--------------------------|-----------|
| Eshelby (dilute)         | \(o(c)\)  |
| Mori-Tanaka              | \(o(c^2)\) |
| Self-consistent          | \(o(c)\)  |
| IDD                      | \(o(c^2)\) |

FIGURE 4 Schematic illustration of the influence of unit cell size. A, Different choices of a unit cell; B, Convergence of different boundary conditions. RVE, representative volume element

Accuracy assessment: In Table 1, we recall the accuracy level of some mean-field methods from the literature, where \(c = \sum_{i=1}^{N} c_i\) denotes the total volume fraction of all inclusions. A function \(f(c)\) is said to be \(o(c^m)\) if there exist two \(c\)-independent positive constants \(A\) and \(m\) such that \(|f(c)| \leq Ac^m\) as \(c \to 0\). The accuracy level given in Table 1 provides a two-step model hierarchy, however, is only restricted to a limit case of a very low inclusion volume fraction \(c \to 0\) and does not have a generality for all possible inclusion volume fractions. Therefore, the special choice for \(n = 0, 1\) in the model hierarchy (46) does not have generality due to the lack of a hierarchical model structure. The choice should be tailored for the problem under study.

Unit cell size: An RVE is defined as a statistical representative of the microstructure of the material under study. The choice of an RVE is not unique, but, by definition, any RVE should return the same effective properties \(\bar{C}\) in Equation (15) or \(\bar{S}\) in Equation (16). However, this is not always practicable, such that, instead of an RVE, a unit cell is used for formulation of the micropbanel (7b), as already mentioned in Section 1. Figure 4A schematically depicts some possible choices of a unit cell for a given microstructure, which do not necessarily meet the requirements of an RVE. With increasing unit cell size, a better estimate of effective properties is expected, as illustrated in Figure 4B for different boundary conditions, see, eg, the work of Fish. Note that Figure 4B is a qualitative illustration, where the relative positions of the different boundary conditions to the exact solution are arbitrarily assumed. In fact, the accuracy of the boundary conditions is not a priori known, eg, for a random composite of a small unit cell size \(n_s\). When unit cell size \(n_s\) is fixed, the linear displacement boundary condition gives the stiffest prediction, whereas the constant traction boundary condition provides the most compliant behavior. In many cases, the periodic boundary condition gives the best prediction, such that the fastest convergence rate may be expected. Of course, it is not generally the case. Hence, the user has the freedom to choose one boundary condition according to his experiences and the specific problem under study. Note also that the convergence rate of a given boundary condition is meant to be its overall performance, but does not necessarily mean that the prediction of a small unit cell size \(n_s\) is more accurate than that for other boundary conditions. The unit cell corresponds to an RVE, when a certain size is reached, such that the exact effective properties can be reproduced. In this work, we consider hierarchical unit cells \(n_s = 1, 2, \ldots\), starting with a basic unit cell \(n_s = 1\) and enlarging their size with an increasing \(n_s\). Additionally, a unit cell of a size \(n_s\) contains all microstructural information of the one of \(n_s - 1\). The hierarchical unit cells are considered within Stage 3 of the aforementioned model hierarchy by means of the FEM. Since a clear hierarchical model structure is obtained by enlarging the unit cell size, this ansatz is quite general.

3.4 | A computable error estimator

Using the enhanced dual solution \(\bar{Z}_n\) of the dual problem (C4) and combining Equations (43), (44), (C1), and (45a), we finally obtain the model error estimate

\[
E_m = \partial_m \left( \bar{u}_h^{(n)} \cdot \bar{Z}_n \right) \approx \int_{\Omega} \bar{e} \left( \bar{Z}_n \right) \bar{\nabla} \left( \bar{u}_h^{(n)} \right) dv =: \bar{E}_m
\]  

(47)
and the discretization error estimate

\[ E_h = \bar{\sigma}_h \left( \bar{u}_h^{(n)} \cdot \bar{z}_h - \pi \bar{z}_h \right) \]

\[ \approx F (\bar{z}_h + \pi \bar{z}_h) - \int_{\Omega} \bar{\sigma} \left[ \bar{z}_h + \pi \bar{z}_h \right] : \left( \bar{C}^{(n)} \bar{u}_h \right) \, dv =: \bar{E}_h, \]

(48)

respectively. The local error indicators \( \eta_m^e \) and \( \eta_h^e \) for each single element \( e \) are then obtained from the corresponding element contributions of their global counterparts (47) and (48), respectively, ie,

\[ \bar{E}_m = \sum_{e=1}^{N_e} \eta_m^e, \quad \eta_m^e = \int_{\Omega} \bar{\sigma} \left[ \bar{z} h + \pi \bar{z}_h \right] : \left( \bar{C}^{(n)} - \bar{C}^{(n+1)} \right) \bar{u}_h \, dv, \]

(49a)

\[ \bar{E}_h = \sum_{e=1}^{N_e} \eta_h^e, \quad \eta_h^e = - \int_{\Omega} \bar{\sigma} \left[ \bar{z}_h + \pi \bar{z}_h \right] : \left( \bar{C}^{(n)} \bar{u}_h \right) \, dv, \]

(49b)

\[ \bar{E} := \bar{E}_m + \bar{E}_h, \]

(49c)

where \( \bar{\Omega} = \bigcup_{e=1}^{N_e} \Omega_e \). In Equation (49c), we introduce \( \bar{E} \) as an error estimate of the total error \( E \) in Equation (36). For the second equation in Equation (49b), the load term \( \bar{F} \) in Equation (48) is neglected for a localization. This does not have any influence on the effectivity for a displacement-controlled approach in Section 4, where \( \bar{F} (\bar{z}_h + \pi \bar{z}_h) = 0 \). Otherwise, for an effectivity improvement, one could use the Galerkin orthogonality

\[ \bar{F} (\bar{z}_h) - \int_{\Omega} \bar{\sigma} \left[ \bar{z}_h \right] : \left( \bar{C}^{(n)} \bar{u}_h \right) \, dv = 0, \]

(50)

which suggests to solve the primal problem (35) on an enhanced FE-space \( \bar{\mathcal{V}}_h \) for an enhanced primal solution \( \bar{u}_h^{(n)} \). In this manner, the load term \( \bar{F} \) can be equivalently replaced by the second term in Equation (50), which can be easily localized into its element contributions. For a numerical efficiency, the patch recovery\(^{61,63} \) can be used to approximate the enhanced primal problem (50) in a similar manner as for the enhanced dual solution \( \bar{z}_h \) in Appendix C.

The sign of \( \eta_m^e \) and \( \eta_h^e \) in Equations (49) indicates the direction of the deviation w.r.t. the quantity of interest \( Q \); hence, only their absolute values are considered as local indicators in the adaptive algorithm, which will be described in the subsequent section.

### 3.5 Adaptive algorithm

For both model and discretization errors to be controlled in a systematic and automated manner, we adopt Algorithm 1.

#### Algorithm 1 Adaptive algorithm

Initialization: set the initial mesh \( \mathcal{T}_{h0} \) with the initial (uniform) elastic property \( \bar{C}^{(n=0)} \) and adaptive step \( i = 0 \); Define a stopping criterion \( \bar{E} = \bar{E}_h + \bar{E}_m \leq TOL \) for the adaptive refinement loop, where \( TOL \) is a user-defined threshold value related to the desired accuracy;

while \( \bar{E} = \bar{E}_h + \bar{E}_m > TOL \) do

| Solve the computable working model problem (35) with (45b); |
| Solve the approximate dual problem (C3) on the current mesh and compute the enhanced dual solution \( \bar{z}_h \) in Equation (C4) using the patch recovery technique \(^{61,63} \); |
| Compute the local fine models \( \bar{C}^{(n_e)} \); |
| Compute the error representations \( \eta_m^e, \eta_h^e, \bar{E}_m, \bar{E}_h \) and \( \bar{E} \) according to the equations (47), (48) and (49); |
| Adaptive refinement: a fixed refinement ratio, such as \( \alpha = 3\% \), of the elements with the largest \( | \eta_h^e | \) and \( | \eta_m^e | \) is spatially refined and enhanced by \( \bar{C}^{(n_e)} \rightarrow \bar{C}^{(n+1)} \), respectively; update the local hierarchical order \( n_e \rightarrow n_e^+ \) for enhanced elements and adaptive step \( i \rightarrow i + 1 \). |

end
For linear elasticity, the effective properties need to be computed only once for a certain microstructure. For macroscopically homogeneous materials, in each adaptive step $i = 0, 1, 2, \ldots$, the (maximal reachable) fine model $\mathbf{C}^{(n^*+i+1)}$ is computed only once for all and stored for a possible call by subsequent steps. The computational cost cannot be saved in this manner, when the considered material is macroscopically heterogeneous, see, eg, a random composite in Section 4.3, or when the mechanical problem is coupled to an additional problem such as phase transformation.

4 | NUMERICAL EXAMPLES

4.1 | Preliminaries

In this section, a compact tension (CT) specimen is investigated, where no crack is assumed. As shown in Figure 5A, we consider a half model. The specimen is stretched by a displacement $\mathbf{u}^* = 0.01$ mm in the vertical direction, which is uniformly distributed on the entire boundary of the hole. The indices 1 and 2 represent the horizontal and the vertical direction, respectively. We restrict ourselves to a two-dimensional case following the notations given in Appendix D, where a plane strain state is assumed.

The specimen is made of a composite material, consisting of a matrix material and fibers of respective properties given in Table 2. In the subsequent examples, we will consider two different classes of materials as follows.

- **Periodic composite**: The macrostructure is made of a periodic repetition of the microstructure. As illustrated in Figure 6A, the basic unit cell with $n_s = 1$ is assumed to be a square matrix (white) with a centrally located circular fiber (black). Higher-order unit cells ($n_s > 1$) are generated by a repetition of the basic unit cell in such a way that the

---

**TABLE 2** Summary of material parameters

| Young's modulus $E$ [MPa] | Poisson's ratio $\nu$ [-] |
|---------------------------|---------------------------|
| Matrix $7 \cdot 10^4$     | 0.25                      |
| Fiber $7 \cdot 10^5$      | 0.25                      |

---

**FIGURE 5** A compact tension specimen in linear elasticity. A, Geometry and boundary conditions; B, Initial mesh [Colour figure can be viewed at wileyonlinelibrary.com]

**FIGURE 6** Artificial generation of hierarchical unit cells. A, Periodic composite; B, Random composite
same number \( n_s \) of basic unit cells is contained for both rows \( i \) and columns \( j \). In this manner, any unit cell with \( n_s > 1 \) remains a square and automatically contains all microstructural information of the one with \( n_s - 1 \). Since size effects (in the context of generalized continuum mechanics\(^{19}\)) are not considered by the present approach, the absolute size of the unit cell does not play a role for computation of the effective properties. For this reason, a specification of the volume fraction of the fibers \( c_f \) suffices for a microscopic geometric description in this case. Due to the fiber arrangement in Figure 6A, the resulting effective material is orthotropic.

- **Random composite**: It contains randomly distributed fibers. Local periodicity is assumed such that homogenization schemes apply. As illustrated in Figure 6B, the fibers are randomly deviated from the center position, such that the effective properties can be expected to be isotropic. For simplicity, the deviations are controlled in such a way that the fibers do not cross the boundaries of the square unit.

In order to solve the underlying microproblem (7b), we will consider the following two classes of methods:

- **Mean-field methods**: Eshelby (B3), Mori-Tanaka (B9), self-consistent (B12), and IDD (B14) in Section 2.3.1;
- **Full-field methods**: FEM (linear displacement) in Equation (A4), FEM (constant traction) in Equation (A5), and FEM (periodic) in Equation (A7) in Section 2.3.2.

Algorithm 1 starts with the initial mesh \( \mathcal{V}_{h0} \) shown in Figure 5B, consisting of linear triangular elements, and with a uniform model distribution \( n(x) = \text{const.} = 0 \). An artificial constraint is added to avoid a mesh refinement around the hole boundary for two reasons, ie, (1) the hole is made for imposing a load and does not correspond to our investigation region; and (2) this avoids a varying mesh quantity for reproducing the hole geometry, thus enabling a pure effectiveness study of our error estimate (49a).

To illustrate the power of goal-oriented adaptivity, we define the quantity of interest \( Q \) as a local type quantity

\[
Q := \int_\Omega \sigma_{ij} dv,
\]

where \( \sigma_{ij} \) represents coefficients of the macrostress tensor \( \sigma \). For this work, we choose \( i = j = 2 \). Furthermore, \( \Omega \) is a local domain out of the whole domain \( \Omega \), ie, the green area marked in Figure 5A, with \( r = 4 \text{ mm} \).

For an effectiveness study of the proposed adaptive approach, we introduce an accurate estimate of the exact global error \( E_i \) in Equation (36), called the actual error \( \hat{E}_i \), as

\[
E_i = Q - Q_{h}^{(n,i)} \approx Q_{\text{ref}} - Q_{h}^{(n,i)} =: \hat{E}_i, \quad i = 0, 1, \ldots, N_s.
\]

Here, \( Q_{h}^{(n,i)} \) represents the quantity of interest computed on the current \( (i) \) mesh with a corresponding \( (i) \) model distribution, where \( N_s \) denotes the number of adaptive refinement steps. Furthermore, \( Q_{\text{ref}} \) represents a reference solution, which is independent of \( i \). Additionally, we introduce a relative actual error

\[
\hat{E}_{rel}^i := \frac{\hat{E}_i}{Q_{\text{ref}}},
\]

and a relative error estimate

\[
\hat{E}_{rel}^i := \frac{\hat{E}_i}{Q_{\text{ref}}},
\]

respectively.

### 4.2 Example 1: periodic composite

In this example, we deal with the periodic composite illustrated in Figure 6A. The volume fraction of the fibers is assumed to be \( c_f = 40\% \).

**4.2.1 Example 1.1: model hierarchy**

Figure 7 shows several hierarchical unit cells discretized with linear triangular elements for the FEM with different microboundary conditions (A4), (A5), and (A7). Using the mesh in Figure 7C, different results are obtained for different boundary conditions, as exemplarily shown in Figure 8 for contour plots of the von Mises stresses \( \sigma_v \) under a pure shear.
FIGURE 7  Example 1.1: A sequence of FE-discretized unit cells with different sizes $n_s$. A, $n_s = 1$; B, $n_s = 2$; C, $n_s = 3$

FIGURE 8  Example 1.1: Contour plots of von Mises stress $\sigma_v$ [MPa] under different microboundary conditions (deformation scaling factor of 10). A, Linear displacement via Equation (A4); B, Constant traction via Equation (A5); C, Periodic via Equation (A7)

loading $\varepsilon_{12} = 0.005$. A maximum von Mises stress is locally achieved by the linear displacement boundary condition (A1), whereas a periodic stress distribution is ensured by the periodic boundary condition (A3) as expected. Additionally, the stress distribution obtained by the constant traction boundary condition (A2) is quite similar to that for the periodic boundary condition.

As stated in Section 4.1, different methods are used to obtain the effective elasticity matrix $\bar{C}$ in Equation (D1). As the considered effective material is orthotropic, the effective moduli $\bar{K}$, $\bar{G}_1$, and $\bar{G}_2$ defined in Equation (D4) are shown in Figures 9A to 9C, respectively, where we consider the unit cell size $n_s$. Since all four mean-field methods, ie, Eshelby (B3), Mori-Tanaka (B9), self-consistent (B12), and IDD (B14), are not able to account for unit cell size effect, their courses remain constant versus $n_s$ in Figure 9. Moreover, Eshelby (B3), Mori-Tanaka (B9), and self-consistent (B12) method are not able to consider the fiber distribution, thus leading to isotropic predictions of effective properties, as can be seen from a comparison between Figures 9B and 9C for $\bar{G}_1 = \bar{G}_2$, which is not the case for the FEM. As discussed in B.4, the IDD method may account for ellipsoidal distribution, which does not correspond to the present case. The underlying inclusion-matrix cell is assumed to be of the same shape of the corresponding inclusion, leading to an isotropic prediction of effective properties. As a result, the IDD estimate coincides with the Mori-Tanaka one as also reported, eg, in the works of Du and Zhang. Interestingly, the Eshelby estimate performs very well when compared to the FEM for the effective shear modulus $\bar{G}_2$ in Figure 9C, whereas a relative large deviation can be observed for the effective moduli $\bar{K}$ and $\bar{G}_1$ in Figures 9A and 9B, respectively. Additionally, its prediction becomes poor, running outside of the Reuss bound, for a higher fiber concentration like $c_f > 50\%$.

As depicted in Figures 9A to 9C, using the FEM, the linear displacement boundary condition (A1) provides an upper bound of the effective elastic moduli, whereas the constant traction one (A2) renders a lower bound. With increasing unit cell size $n_s$, the bounds become narrower. Most strikingly, the estimate made by the periodic boundary condition (A3) lies between the bounds and holds constant with increasing unit cell size $n_s$. In this case, it stays rather close to the lower bound (the constant traction boundary condition) for the effective shear modulus $\bar{G}_2$ in Figure 9C, which is quite reasonable due to the similar stress distributions in Figures 8B and 8C for a pure shear loading. In contrast to that, Figure 9B shows
that the periodic estimate is very close to the upper bound (the linear displacement boundary condition) for the effective shear modulus $G_1$, whereas the periodic estimate approximately lies in the middle of the bounds for the effective bulk modulus $K$ in Figure 9A. Most importantly, as illustrated in Figure 9, the basic unit cell $n_x = 1$ can be used along with the periodic boundary condition to compute an accurate estimate of the effective elasticity matrix $\bar{C}$ at a comparably low computational cost. Once a periodic boundary condition is chosen, there is no need to enlarge the unit cell size $n_x$ for an accuracy improvement. This illustrates the power of the periodic boundary condition for periodic composites. Note that the effective elasticity matrix $\bar{C}$ obtained by the FEM (periodic) in Equation (A7) is still not exact due to the discretization errors.

Correspondingly, we establish the model hierarchy in Equation (46), which is illustrated for the effective elastic moduli $\bar{K}$, $\bar{G}_1$, and $\bar{G}_2$ in Figures 10A to 10C, respectively. For $n = 0$ and $n = 1$, mean-field methods are used, whereas a switch to full-field methods is followed by $n \geq 2$. Compared to the results of full-field methods, a large deviation is observed for the basic model (self-consistent) $n = 0$, which is significantly enhanced by the IDD estimate $n = 1$. At the expense of a much larger computational effort, the IDD estimate is further enhanced by a full-field approximation via the FEM for a basic unit cell problem $n_x = 1$ or $n = 2$. As discussed earlier, since a periodic boundary condition is chosen, no further accuracy improvement can be made by enlarging the unit cell size $n_x$ for $n > 2$. 

**FIGURE 9** Example 1.1: Comparison between different methods for different unit cell sizes $n_x$. 

(A) 

(B) 

(C)
4.2.2 Example 1.2: pure model adaptivity

Based on the model hierarchy in Equation (46), we investigate a special case of pure model adaptivity on the initial mesh in Figure 5B, which is not refined during the adaptive approach. For an effectiveness study, we introduce an estimate of the exact model error $E_m^i$ in Equation (44), called the actual model error $\tilde{E}_m^i$, as

$$E_m^i \approx Q_h,ref - Q_h^{(n)},i = \tilde{E}_m^i, \quad i = 0, 1, \ldots, N_s. \quad (55)$$

Here, $Q_h^{(n)},i$ represents the quantity of interest computed on the initial mesh with the $i$th model distribution, where $N_s$ denotes the number of adaptive refinement steps. Furthermore, $Q_h,ref$ represents a reference solution, which is computed on the initial mesh in Figure 5B with a uniform model distribution $n(\vec{x}) = const. = 2$. Similarly to Equations (53) and (54), we introduce a relative actual model error

$$\tilde{E}_m^i,rel := \frac{\tilde{E}_m^i}{Q_h,ref}, \quad (56)$$

and a relative model error estimate

$$E_m^i,rel := \frac{E_m^i}{Q_h,ref}, \quad (57)$$

respectively. The adaptive approach is stopped until the actual model error $\tilde{E}_m^i$ completely vanishes, where $N_s = 86$ adaptive steps are needed. Exemplarily, Figures 11A to 11C show several distributions of the local model errors $|\eta_m^i|$ in Equation (49a) for different adaptive steps, whereas the resulting model distributions are depicted in Figures 11D to 11F, respectively. In the course of the adaptive model refinements, the local model errors $|\eta_m^i|$ are balanced and significantly reduced.
**FIGURE 11** Example 1.2: Results of pure model adaptivity – Part I. A, $i = 1$; B, $i = 7$; C, $i = 14$; D, $i = 1$; E, $i = 7$; F, $i = 14$; G, $|\hat{E}_{m,rel}| = 11\%$; H, $|\hat{E}_{m,rel}| = 0.91\%$; I, $|\hat{E}_{m,rel}| = 0.23\%$

**FIGURE 12** Example 1.2: Results of pure model adaptivity – Part II. A, Quantities of interest $Q^{(n)}_{h,i}$ and $Q_{h,ref}$; B, Relative errors $\hat{E}_{m,rel}$ and $\tilde{E}_{m,rel}$ [Colour figure can be viewed at wileyonlinelibrary.com]

Furthermore, Figure 12A shows the quantity of interest $Q^{(n)}_{h,i}$ versus adaptive steps, where a convergence to the reference value $Q_{h,ref}$ can be clearly observed. For a numerical efficiency of a structural analysis, it is preferable to limit the use of the FEM for the underlying unit cell computation as strongly as possible. Figure 12B depicts the relation between the faction $c_{fem}$ of elements using the FEM and the relative actual model error $\hat{E}_{m,rel}$, where a comparison to the relative model error estimate $\tilde{E}_{m,rel}$ is additionally given. The reduction of the relative actual model error $\hat{E}_{m,rel}$ is rapid at the beginning for $c_{fem} < 30\%$, then becomes somewhat slower until a sudden jump to zero for $c_{fem} = 100\%$. The relative model error estimate
\( \tilde{E}_{m,rel} \) somewhat underestimates the relative actual model error \( \hat{E}_{m,rel} \), but with a very good effectivity. Additionally, \( \hat{E}_{m,rel} \) correctly predicts the sign of \( \tilde{E}_{m,rel} \) except for only 2 out of 86 adaptive steps at the end of the model refinements. Most strikingly, the zero actual model error \( \hat{E}_{m,rel} = 0 \) for \( c_{\text{fem}} = 100\% \) is reproduced by \( \tilde{E}_{m,rel} \) to working precision. Finally, Figures 11G to 11I show several model distributions obtained by the adaptive approach for different error levels. We observe that the actual model error \( \hat{E}_{m,rel} \) can be reduced from 26.4% for the initial step to 0.24% by a use of the FEM in a comparably small region, showing the effectiveness of the proposed adaptive approach.

### 4.2.3 Example 1.3: coupled model and mesh adaptivity

Now, we consider a fully coupled adaptivity using Algorithm 1, where model adaptivity and adaptive FEM are simultaneously applied. Local model error indicators \( |\eta_{m}^{e}| \) and local discretization error indicators \( |\eta_{d}^{e}| \) in Equation (49) are depicted in Figures 13A to 13C and Figures 13G to 13I for different adaptive steps, respectively. In the course of the adaptive refinements, both of them are balanced and significantly reduced. The balance effect is weaker around the hole due to the artificial constraint avoiding a mesh refinement there, see Figures 13H and 13I. As shown in Figures 13J to 13L, the local mesh refinements are mainly located within the local domain \( \overline{\Omega} \) in the quantity of interest (51). Similar trends can also be found for model refinements shown in Figures 13D to 13F. Since Algorithm 1 aims at a balanced model error distribution, as a coupling effect to the adaptive mesh refinements, the model on coarsest meshes (sooner or later) starts to be refined, as can be seen from Figure 13F. Compared to Figures 11D to 11F for a pure model adaptivity, Figures 13D to 13F show a different model refinement pattern due to the coupling effect with the adaptive mesh refinements. More precisely, the mesh adaptivity results into a varying distribution of element size, which has a further influence on the model error distribution. Additionally, a hierarchical order \( n > 2 \) is not achieved, since it does not provide any accuracy improvement to the model \( n = 2 \) due to the periodic boundary condition. This is also reflected by the local model error distributions in Figures 13B and 13C, where \( \eta_{h}^{e} = 0 \) holds for regions using the model \( n = 2 \) (yellow regions in Figures 13E and 13F).

Figure 14A shows the quantity of interest \( Q_{W}^{cf} \) versus adaptive steps, where a convergence to a reference value \( Q_{\text{ref}} \) can be clearly observed. The reference value \( Q_{\text{ref}} \) is obtained by using a mesh, which is refined uniformly from the last adaptive mesh in Figure 13L, with a uniform model distribution \( n(\overline{x}) = \text{const.} = 2 \). In Figure 14B, the relative actual error \( \hat{E}_{rel}^{i} \) in Equation (53) is shown to be effectively reduced by the adaptive approach, where an additional comparison to the relative error estimate \( \tilde{E}_{rel}^{i} \) in Equation (54) is given. The error estimate \( \tilde{E}_{rel}^{i} \) appears to somewhat underestimate the actual error \( \hat{E}_{rel}^{i} \) and is able to mimic the decreasing trend of the actual error \( \hat{E}_{rel}^{i} \). These observations are quite similar to those obtained from our previous work\(^{53}\) for a different model hierarchy, where a more detailed discussion on the error estimator was given. Finally, Figures 13M to 13O show several model distributions obtained by the adaptive approach for different error levels. We observe that the actual error \( \hat{E}_{rel} \) can be reduced from 35.9% for the initial step to 4.61% by a use of the FEM in a comparably small region, confirming the effectiveness of the proposed adaptive approach. Compared to Figures 11G to 11I for a pure model adaptivity, a different model refinement pattern is obtained here due to the coupling effect with the adaptive mesh refinements, as already discussed above.

### 4.3 Example 2: random composite

In this example, we deal with the random composite illustrated in Figure 6B. The distribution of the fiber volume fraction \( c_{f} \) is macroscopically random and assumed to satisfy some statistical properties like the statistical mean \( \text{mean}(c_{f}) = 20\% \) and the standard deviation \( \text{dev}(c_{f}) = 0.012 \). For a larger phase contrast, we change Young’s modulus of the fiber in Table 2 to \( 1.4 \cdot 10^{6} \) MPa. We consider one specific realization shown in Figure 15A for 357 given sampling points. Additionally, the distribution of fibers is random for each sampling point, as exemplarily shown for the sampling points \( A, B, \) and \( C \) in Figures 15B to 15D, respectively. This sampling procedure is done once for all the following FE computations and serves as a basis for determining the underlying microstructure for each macroelement. In our calculations, the underlying microstructure for each element is assumed to be the same as of the sampling point with the nearest distance from the element center. Furthermore, all fibers are assumed to have a same diameter, such that different volume fractions can be reached by adapting the size of the matrix. As for Example 1, the model hierarchy in Equation (46) is used. Despite of the random composite rather than a periodic one, the periodic boundary condition (A3) is chosen for a fast convergence rate, as depicted in Figure 16A and Figure 16B for the effective moduli \( \overline{K} := (\overline{C}_{11} + \overline{C}_{22} + 2 \cdot \overline{C}_{12})/4 \) and \( \overline{G} := (\overline{C}_{11} - \overline{C}_{12} + 2 \cdot \overline{C}_{44})/4 \), respectively. The aforementioned nonstandard definitions are due to the fact that the effective properties obtained from the FEM are not perfectly isotropic.

On this basis, as for Example 1.3, we consider a fully coupled adaptivity using Algorithm 1. For an investigation of hierarchical unit cells, a larger refinement ratio \( \alpha = 6\% \) is used. Local model error indicators \( |\eta_{m}^{e}| \) and local discretization
FIGURE 13  Example 1.3: Results of coupled adaptivity – Part I. A, $i = 1$; B, $i = 7$; C, $i = 14$; D, $i = 1$; E, $i = 7$; F, $i = 14$; G, $i = 1$; H, $i = 7$; I, $i = 14$; J, $i = 1$; K, $i = 7$; L, $i = 14$; M, $|\hat{E}_{\text{rel}}| = 14.1\%$; N, $|\hat{E}_{\text{rel}}| = 7.68\%$; O, $|\hat{E}_{\text{rel}}| = 4.61\%$

error indicators discretization error $|\eta^e_h|$ in Equation (49) are depicted in Figures 17A to 17C and Figures 17G to 17I for different adaptive steps $i$, respectively. In the course of the adaptive refinements, both of them are balanced and significantly reduced. The balance effect is weaker around the hole due to the artificial constraint avoiding a mesh refinement there, see Figures 17H and 17I. As shown in Figures 17J to 17L, the local mesh refinements are mainly located within the local domain $\tilde{\Omega}'$ in the quantify of interest (51) at the beginning and then spread to surrounding regions for a balanced discretization error distribution. Similar trends can also be found for model refinements shown in Figures 17D to 17F. A maximal hierarchical order $n = 10$ is achieved in Figure 17F for a very small region, whereas, for a comparably large
FIGURE 14  Example 1.3: Results of coupled adaptivity – Part II. A, Quantities of interest $Q^{(n,i)}_q$ and $Q_{ref}$; B, Relative errors $\hat{E}_{rel}$ and $\tilde{E}_{rel}$.

[Colour figure can be viewed at wileyonlinelibrary.com]

FIGURE 15  Example 2: Illustration of a random composite. A, Heterogeneous distribution of the fiber volume fraction $c_f$ on chosen sampling points; B, Point A for $n_s = 4$; C, Point B for $n_s = 4$; D, Point C for $n_s = 4$.

FIGURE 16  Example 2: Illustration of hierarchical models for different sampling points.
region, a unit cell \( n = 3 \) of a small size \( n_\epsilon = 2 \) suffices to consider hierarchical unit cells. This illustrates the power of the periodic boundary condition even for the random composite under study.

For an effectiveness study, Figure 18A shows the quantity of interest \( Q_{\text{ref}}^{(n_\epsilon)} \) versus adaptive steps, where a convergence to the reference value \( Q_{\text{ref}} \) can be clearly observed. Here, \( Q_{\text{ref}} \) is obtained by using a mesh, which is refined uniformly once from the last adaptive mesh in Figure 17L, with a uniform model distribution \( n(\vec{x}) = \text{const.} = 5 \). In Figure 18B, the relative actual error \( \hat{E}_{\text{rel}} \) in Equation (53) is shown to be effectively reduced by the adaptive approach, where an additional comparison to the relative error estimate \( \tilde{E}_{\text{rel}} \) in Equation (54) showing a good effectivity is given. Additionally, Figures 17M to 17O depict several model distributions obtained by the adaptive approach for different error levels, showing that the actual error \( \hat{E}_{\text{rel}} \) can be reduced from 22.2% for the initial step to 3.66% by a use of the FEM in a comparably small region.

**FIGURE 17** Example 2: Results of coupled adaptivity – Part I. A, \( i = 1; B, i = 7; C, i = 14; D, i = 1; E, i = 7; F, i = 14; G, i = 1; H, i = 7; I, i = 14; J, i = 1; K, i = 7; L, i = 14; M, |\hat{E}_{\text{rel}}| = 11.22%; N, |\hat{E}_{\text{rel}}| = 5.03%; O, |\hat{E}_{\text{rel}}| = 3.66%
FIGURE 18  Example 2: Results of coupled adaptivity – Part II. A, Quantities of interest $Q_h^{ref}$ and $Q_{ref}$; B, Relative errors $\hat{E}_{rel}$ and $\tilde{E}_{rel}$ [Colour figure can be viewed at wileyonlinelibrary.com]

A similar model refinement pattern as for Example 1.3 in Figures 17M to 17O is obtained here due to the coupling effect with the adaptive mesh refinements. The effectiveness of the proposed adaptive approach is confirmed again.

In view of a numerical efficiency, compared to a uniform model distribution $n(\mathbf{x}) = \text{const.} = 2$, the model distributions in Figures 17M to 17O achieve a speed-up factor of 16, 7.4, and 2.2, respectively.

5 | CONCLUSION AND OUTLOOK

This work presents a continuation of our previous work\textsuperscript{63} by considering two major concerns arising in homogenization of linear elastic heterogeneous materials.

- The need for a full-field approximation obtained by a computational method (here FEM) where an analytical (mean-field) method does not suffice for the pursued accuracy level.
- An adaptive selection of unit cell size for a further accuracy improvement of computational methods.

We have shown that these two concerns can be simultaneously addressed by an appropriately formulated model hierarchy within the framework of goal-oriented adaptivity. This has been achieved by interpreting the mean-field and full-field methods as different approximations of full-field formulations. Three typical microboundary conditions have been examined and suggested to be chosen prior to the adaptive approach. Considering both model and discretization errors, the proposed adaptive approach has been shown to be effective for two different classes of materials. Compared to a uniform FE$^2$ approach, a promising speed-up factor is achieved by the model distribution obtained from model adaptivity.

Clearly, we are still on the initial stage of development, firstly aiming at simplest problems like linear elasticity. However, the proposed methodology provides a basis for an extension to nonlinear homogenization problems, like large deformations or plasticity, for future work. An extension to three-dimensional problems is of practical importance, however, would be straightforward without any theoretical gains. Model adaptivity for reduced-order homogenization schemes is of our particular interest. Our previous work\textsuperscript{68} developed an adaptive reduced order homogenization scheme on an empirical basis. For an error control, a framework of goal-oriented adaptivity should be incorporated in future. Furthermore, an eventual mathematical proof of the assumption in Figure 3B is another challenging task.

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APPENDIX A

MICROBOUNDARY CONDITIONS

In the following, we consider three different microboundary conditions.

A.1 | Continuous formulation

The following three microboundary conditions are consistent with the Hill-Mandel condition (10c).

1. Linear displacement boundary condition: As depicted in Figure A1B, this Dirichlet-type boundary condition takes the form

\[ u(x) = \bar{\varepsilon} x, \quad \forall x \in \Gamma. \]  

(A1)

2. Constant traction boundary condition: As shown in Figure A1C, a Neumann-type boundary condition is established by

\[ t(x) = \bar{\sigma} n(x), \quad \forall x \in \Gamma, \]  

(A2)

where \( n \) is the outward normal vector at the microboundary point \( x \in \Gamma \).

3. Periodic boundary condition: As illustrated in Figure A1D, whereas the entire boundary is decomposed into two parts \( \Gamma = \Gamma^+ \cup \Gamma^- \) with associated point pairs \( x^+ \in \Gamma^+ \) and \( x^- \in \Gamma^- \), we assume periodic displacements and antiperiodic tractions on \( \Gamma \) as

\[ u(x^+) - u(x^-) = \bar{\varepsilon}(x^+ - x^-), \]  

(A3a)

\[ t(x^+) + t(x^-) = 0, \quad \forall x^+ \in \Gamma^+, x^- \in \Gamma^-, \]  

(A3b)

respectively. Equation (A3a) guarantees the kinematical conformity of the deformed boundary with neighboring RVEs, whereas the statical equilibrium is ensured by Equation (A3b).

A.2 | FE implementation

Proceeding from the weak formulation (32), we briefly outline the implementation of the microboundary conditions. For detailed FE algorithms, the interested reader is referred to the works of Miehe and Koch\(^{69}\) and Perić et al.\(^{70}\)

1. Linear displacement boundary condition: the load term in Equation (32) vanishes, ie, \( F(\delta u) = 0 \). Formally, we have

\[ \varphi (u; \delta u) = -B(u; \delta u) = 0, \quad \forall \delta u \in \Gamma^0, \]  

(A4)

with the constraint (A1).

2. Constant traction boundary condition: using Equation (A2), the load term in Equation (32) becomes

\[ F(\delta u) = \int_{\Gamma} \delta u \cdot \bar{\sigma} \cdot n dA. \]  

(A5)
Note that, for a strain-driven approach, additional effort has to be paid to ensure a prescribed macrostrain $\bar{\varepsilon}$ instead of $\bar{\sigma}$, see, eg, the work of Miehe and Koch for an approach based on Lagrange multipliers.

3. **Periodic boundary condition**: with the strain polarization $\varepsilon = \bar{\varepsilon} + \tilde{\varepsilon}$ in mind, where $\tilde{\varepsilon}$ is a fluctuation part, we correspondingly split the microdisplacement vector into two part, ie, $u(x) = u^0(x) + \tilde{u}(x)$, where $u^0 = \bar{x}$. In this manner, using Equation (10a), the primal microproblem (7b) or (32) becomes an equivalent eigenstrain problem of the strong form

$$\begin{cases}
\text{Div}(\sigma) = \text{Div} \left( C \left( \bar{\varepsilon} + \varepsilon \right) \right) = 0, & \text{in } \Omega \\
\langle \tilde{\varepsilon} \rangle = 0,
\end{cases}$$

and of the weak residual form

$$\varrho(\tilde{u}; \delta \tilde{u}) = -\int_{\Omega} \tilde{\varepsilon} [\delta \tilde{u}] : C(\bar{\varepsilon} + \varepsilon) dV = 0, \quad \forall \delta \tilde{u} \in \hat{V},$$

where $F(\delta \tilde{u}) = 0$. Note that the fluctuation part of the microdisplacement vector $\tilde{u}$ is the primal solution of the eigenstrain problem (A7), whereas the homogeneous part $u^0$ constitutes the constant eigenstrain $\bar{\varepsilon}$. Then, we split the microdisplacement vector into three parts as $u(x) = [\tilde{u}^{in} \tilde{u}^+ \tilde{u}^-]$. While $\tilde{u}^{in}$ corresponds to the displacement in the interior domain, $\tilde{u}^+$ and $\tilde{u}^-$ are the displacements at $x^+ \in I^+$ and $x^- \in I^-$, respectively. On this basis, we arrive at an alternative version of (A3a)

$$\tilde{u}^+(x^+) = \tilde{u}^-(x^-).$$

In the context of the FEM, the combination of Equations (A7) and (A8) leads to a reduced equation system for solving $\tilde{u}^{in}$ and $\tilde{u}^+_h$, see, eg, the work of Perić et al. for details.

**APPENDIX B**

**SEVERAL WELL-ESTABLISHED MEAN-FIELD METHODS**

In the following, we describe some well-established mean-field methods by specifying the single inclusion problem in Figure 2B.

**B.1 Eshelby (dilute) method**

Typically, in micromechanics, a prescribed macrostrain tensor $\bar{\varepsilon}$ is ensured by the linear displacement boundary condition (A1), whereas a prescribed macrostress tensor $\bar{\sigma}$ is imposed by the traction boundary condition (A2). The Eshelby method...
considers the single inclusion problem in Figure 2B by defining
\[ C' := C_0, \quad \epsilon' := \epsilon, \]  
where the inclusion interaction is completely neglected. It follows from Equation (29) that
\[ \Delta_i^{\text{dilute}} = \left( I^S + S_0^{-1} C_0^{-1} (C_i - C_0) \right)^{-1}, \]  
where \( S_0^0 \) is the Eshelby tensor depending on the matrix material property \( C_0 \) and the shape of the inclusion \( i \). Inserting Equation (B2) into Equation (22a) renders the dilute estimate of \( C \) as
\[ C^{\text{dilute}} = C_0 + \sum_{i=1}^{N} C_i (C_i - C_0) \left( I^S + S_0^{-1} C_0^{-1} (C_i - C_0) \right)^{-1}. \]  
Alternatively, one may proceed with Equation (A2) and have \( \sigma' = \sigma \). Then, it follows from Equation (31) that
\[ B_i^{\text{dilute}} = \left( S_i - S_0 \left( S_i - S_0 \right) \right)^{-1} S_0, \]  
together with Equation (22b), leading to the dilute estimate of \( S \) as
\[ S^{\text{dilute}} = S_0 + \sum_{i=1}^{N} C_i (S_i - S_0) \left( S_i - S_0 \left( S_i - S_0 \right) \right)^{-1} S_0. \]  
It is not difficult to identify \( C^{\text{dilute}} \neq I^S \), such that the dilute estimate is not reciprocal-invariant. In other words, the dilute method gives different predictions on effective properties, depending on the applied boundary conditions (A1) or (A2). In contrast to that, the methods introduced in subsequent sections are all reciprocal invariant.

### B.2 | Mori-Tanaka method

To take into account the inclusion interaction, the work of Mori and Tanaka\(^6\) suggests the single inclusion problem in Figure 2B by defining
\[ C' := C_0, \quad \epsilon' := \epsilon_0, \]  
where \( \epsilon_0 \) is the average strain in the matrix material. It is shown that the strain localization tensor for the inclusion \( i \) becomes
\[ \Delta_i^{\text{MT}} = \Delta_i^0 \left( c_0 I^S + \sum_{j=1}^{N} c_j^0 \Delta_j^0 \right)^{-1}, \]  
where the local localization tensor \( \Delta_i^0 \) is defined as
\[ \epsilon_i = \Delta_i^0 \epsilon_0, \quad \Delta_i^0 = \left( I^S + S_i^0 C_0^{-1} (C_i - C_0) \right)^{-1}. \]  
Finally, inserting Equation (B7) into Equation (22a) renders
\[ C^{\text{MT}} = C_0 + \sum_{i=1}^{N} C_i (C_i - C_0) \left( \Delta_i^0 \left( c_0 I^S + \sum_{j=1}^{N} c_j^0 \Delta_j^0 \right)^{-1} \right). \]  

### B.3 | Self-consistent method

The self-consistent method\(^7\) assumes
\[ C' := C, \quad \epsilon' := \epsilon, \]
for the single inclusion problem in Figure 2B, such that Equation (29) becomes

$$A^{SC}_{i} = \left( \mathbf{I}^S + \mathbf{S}_i \left( \mathbf{C}^{SC} \right)^{-1} \left( \mathbf{C}_i - \mathbf{C}^{SC} \right) \right)^{-1},$$  \hspace{1cm} (B11)$$

where $\mathbf{S}_i$ differs from $S^0_i$ by using the effective elasticity tensor $\mathbf{C}^{SC}$ rather than the elasticity tensor of the matrix $\mathbf{C}_0$. Inserting Equation (B11) into Equation (22a) renders the self-consistent estimate of $\mathbf{C}$ as

$$\mathbf{C}^{SC} \mathbf{C} = \mathbf{C}_0 + \sum_{i=1}^{N_i} c_i (\mathbf{C}_i - \mathbf{C}_0) \left( \mathbf{I}^S + \mathbf{S}_i \left( \mathbf{C}^{SC} \right)^{-1} \left( \mathbf{C}_i - \mathbf{C}^{SC} \right) \right)^{-1}. \hspace{1cm} (B12)$$

Clearly, Equation (B12) is an implicit equation, which has to be solved iteratively.

### B.4 Interaction direct derivative

The so-called interaction direct derivative (IDD) method of Du and Zheng\(^8\,67\) possesses the following features.

- It has an explicit structure.
- It is valid for multiphase composites with various inclusion geometries and isotropic or anisotropic properties.
- It accounts for interaction between inclusions and matrix as well as inclusion distributions.

The IDD method is an explicit version of the effective self-consistent method, which is deduced from the generalized self-consistent method.\(^71\) As shown in the work of Zheng and Du,\(^67\) it may be interpreted as the single inclusion problem in Figure 2B with

$$\mathbf{C}' := \mathbf{C}_0, \hspace{1cm} \mathbf{\sigma}' := \mathbf{\sigma}^F = \left( \mathbf{I}^S - \sum_{i=1}^{N_i} \left( c_i C_D \sum_{j=1}^{N_j} ((S_j - S_0)^{-1} + C_j) \right) \right)^{-1} \mathbf{\sigma}. \hspace{1cm} (B13)$$

Here, $C_j$ is the eigenstiffness tensor computed by using the matrix material property $\mathbf{C}_0$ and the geometry of the inclusion $j$, whereas the eigenstiffness tensor $C_D$ is computed by using the matrix material property $\mathbf{C}_0$ and the geometry of the so-called inclusion-matrix cell $D_j$, which is designed to account for inclusion distributions. The effective elasticity tensor of the IDD estimate reads

$$\mathbf{C}^{IDD} = \mathbf{C}_0 + \sum_{j=1}^{N_j} c_j (C_j - C_0) A_j^* S_j^0 \mathbf{S}_0 \mathbf{S}_0^{-1} \sum_{i=1}^{N_i} c_i (C_i - C_0) A_i^*, \hspace{1cm} (B14)$$

where

$$A_i^* = \left( \mathbf{I}^S + S_i^0 C_0^{-1} (C_i - C_0) \right)^{-1}, \hspace{1cm} (B15)$$

and $S^0_i$ is the Eshelby tensor computed by using the matrix material property $\mathbf{C}_0$ and the geometry of the inclusion $i$, whereas the Eshelby tensor $S^0_j$ is computed by using the matrix material property $\mathbf{C}_0$ and the geometry of an inclusion-matrix cell $D_j$. By comparing Equation (B14) with Equation (22a), we conclude that

$$A_i^{IDD} = (C_i - C_0)^{-1} \left( \mathbf{I}^S - \sum_{j=1}^{N_j} c_j (C_j - C_0) A_j^* S_j^0 \mathbf{S}_0 \mathbf{S}_0^{-1} \left( (C_i - C_0) A_i^* \right) \right)^{-1} \left( (C_i - C_0) A_i^* \right). \hspace{1cm} (B16)$$

According to the works of Du and Zheng,\(^8\,67\) the geometry of the inclusion-matrix cell $D_j$ accounts for the inclusion distribution. For anisotropic distributions, additional effort has to be paid to identify the correct geometry of $D_j$. For the orthotropic effective material in Figure 6A, the inclusion-matrix cell would be a square rather than an ellipsoidal, thus violating the requirement of the IDD, i.e., ellipsoidal distribution given in the work of Du and Zheng.\(^8\) For the model hierarchy in Equation (46), the inclusion-matrix cell is assumed to be of the same shape of the corresponding inclusion for simplicity. As shown in Section 4.2, this simplification still provides a sufficient accuracy improvement to the self-consistent estimate in Equation (B12) for the considered example.
APPENDIX C

APPROXIMATIONS FOR A COMPUTABLE ERROR REPRESENTATION

To arrive at a computable error representation based on the exact error representation (44), we make the following three approximations.

1. The exact model of hierarchical order \( n \to \infty \) is replaced by a fine model of a hierarchical order \( n^+ > n \). Hence, we obtain for Equation (43)

\[
\varphi_m(u_h(n) \cdot \bar{z}) \approx \varphi_m'(u_h(n) \cdot \bar{z}) := B^{(n)}(u_h(n) \cdot \bar{z}) - B^{(n^+)}(u_h^{(n)} \cdot \bar{z}). \quad (C1)
\]

2. The exact dual problem (42) also depends on the exact primal solution \( \bar{u} \) and requires knowledge of the exact model. Hence, we introduce an approximate dual problem

\[
B(n)(z_h; \delta \bar{u}) = Q_S(n)(u_h(n), u_h(n); \delta \bar{u}) \quad \text{by the replacements } B \approx B(n), \quad Q_S \approx Q_S(n), \quad \text{and } \bar{u} \approx \bar{u}_h(n), \leq 2 \text{ leading to a linearization of } (42).
\]

3. In practice, the approximate dual problem (C2) is not solved exactly. Instead, a spatially discretized version of (C2), i.e.,

\[
B(n)(z_h; \delta \bar{u}_h(n)) = Q_S(n)(u_h(n), u_h(n); \delta \bar{u}_h(n)), \quad (C3)
\]

is solved via the FEM, using the same mesh as for the primal problem and thus preserving an analogous structure of the primal problem (see, e.g., the work of Widany and Mahnken\textsuperscript{72}). Here, \( \bar{z}_h(n) \) is the FE solution of the approximate dual problem (C2), which is not directly useful for the error representation (44) due to the Galerkin orthogonality. For this reason, we use, in this work, a patch recovery approach developed in our previous works\textsuperscript{61,63} to construct an approximate solution of

\[
B(n)(\bar{z}_h(n); \delta \bar{u}_h(n)) = Q_S(n)(u_h(n), u_h(n); \delta \bar{u}_h(n)), \quad (C4)
\]

on an enhanced FE-space \( \delta \bar{u}_h(n) \in \bar{V}_h(n) \) satisfying \( \bar{V}_h(n) \subset \bar{V}_h(n) \subset \bar{V}_h(n), \) using the hierarchical FE structure by increasing the polynomial interpolation order.

APPENDIX D

SOME NOTATIONS FOR A TWO-DIMENSIONAL IMPLEMENTATION

In the following, we declare some notations used in Section 4. In a two-dimensional case, a matrix representation of Equation (15) takes the form

\[
\vec{\sigma} = \bar{C} \cdot \vec{\varepsilon}, \quad (D1)
\]

or more precisely

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix} =
\begin{bmatrix}
\bar{C}_{11} & \bar{C}_{12} & \bar{C}_{14} \\
\bar{C}_{21} & \bar{C}_{22} & \bar{C}_{24} \\
\text{sym.} & & \bar{C}_{44}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
2 \cdot \varepsilon_{12}
\end{bmatrix}. \quad (D2)
\]

For a plane strain state, we have \( \varepsilon_{33} = 0 \) and \( \sigma_{33} \neq 0 \) for the strain and the stress component normal to the plane, respectively. For an orthotropic material, Equation (D2) reduces to

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{12}
\end{bmatrix} =
\begin{bmatrix}
\bar{C}_{11} & \bar{C}_{12} & 0 \\
\bar{C}_{21} & \bar{C}_{22} & 0 \\
\text{sym.} & & \bar{C}_{44}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
2 \cdot \varepsilon_{12}
\end{bmatrix}. \quad (D3)
\]
For the periodic composite in Figure 6A, the relation $\bar{C}_{11} = \bar{C}_{22}$ holds. Following the line of Pecullan et al.\textsuperscript{33} we define three independent effective material parameters for this two-dimensional case, i.e., a bulk modulus and two shear moduli, as

$$K := (\bar{C}_{11} + \bar{C}_{12})/2,$$

$$\bar{G}_1 := (\bar{C}_{11} - \bar{C}_{12})/2,$$

$$\bar{G}_2 := \bar{C}_{44},$$

respectively. For an isotropic material-like the random composite in Figure 6B, the number of independent effective material parameters further reduces to two, due to the relation $\bar{G}_1 = \bar{G}_2$.\textsuperscript{(D4a)-(D4c)}