A computational framework for homogenization and multiscale stability analyses of nonlinear periodic materials

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Abstract
This article presents a consistent computational framework for multiscale first-order finite strain homogenization and stability analyses of rate-independent solids with periodic microstructures. The homogenization formulation is built on a priori discretized microstructure, and algorithms for computing the matrix representations of the homogenized stresses and tangent moduli are consistently derived. The homogenization results lose their validity at the onset of first bifurcation, which can be computed from multiscale stability analysis. The multiscale instabilities include: (a) microscale structural instability calculated by Bloch wave analysis; and (b) macroscale material instability calculated by rank-1 convexity checks on the homogenized tangent moduli. Implementation details of the Bloch wave analysis are provided, including the selection of wave vector space and the retrieval of real-valued buckling mode from complex-valued Bloch wave. Three methods are detailed for solving the resulted constrained eigenvalue problem—two condensation methods and a null-space projection method. Both the homogenization and stability analyses are verified using numerical examples including hyperelastic and elastoplastic periodic materials. Various microscale buckling phenomena are demonstrated. Aligned with theoretical results, the numerical results show that the microscopic long wavelength buckling can be equivalently detected by the loss of rank-1 convexity of the homogenized tangent moduli.

KEYWORDS
Bloch wave analysis, multiscale stability, nonlinear homogenization, null-space projection method, periodic materials

1 | INTRODUCTION

In recent years, architected materials have received much attention and are expected to have a significant impact on how the materials are designed and discovered in future. By designing the underlying periodic microstructures, the architected materials can achieve desired engineering properties that are often not observed in nature materials, for example, high strength-to-weight ratio,\(^1\) negative Poisson’s ratio,\(^2,3\) desirable band-gaps,\(^4,5\) high energy absorption,\(^6,7\) and so forth. For this reason, architected materials are also known as metamaterials. The progress in metamaterials design and application is also fueled by the advancements of additive manufacturing technologies,\(^8\) through which the fabrication of complex geometries and multiple material phases in materials microstructures is now possible. As a key tool in metamaterials
analysis and design, consistent computational frameworks that are capable of describing metamaterials behavior are crucially needed to realize future metamaterials.

As a bridge between micro and macro scales, the homogenization theories can be dated back to Voigt\textsuperscript{9} and Reuss\textsuperscript{10} bounds, where uniform strain and stress are, respectively, assumed on microscale for the calculation of the homogenized material properties at macroscale. The theories were further developed and refined in a series of work\textsuperscript{11–13} on linear composites. The extension to the nonlinear regime was initiated by the work of Hill\textsuperscript{14} and then followed by Ogden,\textsuperscript{15} Talbot and Willis,\textsuperscript{16} among others.\textsuperscript{17–19} In contrast to the theoretical approaches that are mostly used to estimate bounds on macroscale material properties, the computational approaches to homogenization rely on finite element modeling of a representative volume element (RVE) of the underlying microstructure and are thus capable of capturing the effect brought by detailed geometric features of the microstructure.\textsuperscript{20–22} For random heterogeneous composites, the selection of RVE is not straightforward and usually based on statistical methods.\textsuperscript{23} On the contrary, for periodic (meta)materials, which are also the focus in this study, the definition of RVE is unambiguous and can be chosen simply as the fundamental periodic cell, that is, the unit cell. As a result, computational homogenization methods can be used as a reliable tool for accurate and effective calculation of the overall macroscopic properties of periodic (meta)materials. The transition between the macro and micro scales is governed by the Hill–Mandel condition\textsuperscript{14,24} that states the energy equivalence between the two scales. Extension of this scale transition to incorporate inertia and body forces has been made in Reference 25, where the transition condition is formulated using the principle of multiscale virtual power. On the computational side, efforts have also been made to achieve consistent and efficient algorithms for calculating macroscopic properties (i.e., homogenized stress and tangent moduli), cf. Miehe's work\textsuperscript{22} where these quantities are derived based on discretized microstructures and Lagrange multipliers. In addition, various advancement and development on computational homogenization such as incorporation of multiphysics,\textsuperscript{26} scale effects,\textsuperscript{27} crack modeling on microscale,\textsuperscript{28,29} among others,\textsuperscript{30–32} have been achieved. A comprehensive review on this topic can be found in Reference 33.

An implicit assumption for the homogenization analysis results to be valid resides on the condition that the RVE, which is usually taken to be one unit cell in periodic materials, remains valid for characterizing the response during the loading process. This in turn implies that the principal loading path is stable, and no other bifurcated solution besides the principal solution exists. However, from a structural stability viewpoint, the stability of the periodic microstructures is not always guaranteed. Using homogenization analysis, Abeyaratne and Triantafyllidis\textsuperscript{34} showed that with strong ellipticity (rank-1 convexity) preserved in the matrix material, the homogenized periodic porous solids, however, can still lose strong ellipticity at adequately large loads, which implies a possible formation of the shear band. The shear band formation due to the loss of strong ellipticity has been well studied and understood, see Reference 35. Although it seems plausible that the deformation localization on the macroscale may be initiated by a buckling type instability on the microscale, this stability phenomenon across micro and macro scales was not immediately clear. An early effort toward understanding this issue was made by Triantafyllidis and Maker,\textsuperscript{36} where an analytical study on the bifurcation problem of a layered hyperelastic composite was carried out. This study showed that the macroscopic stable region consistently envelops the microscopic stable region and for the considered composites the loss of ellipticity condition for the homogenized material is the same as the condition for the long wavelength buckling of the microstructure. Subsequent work by Geymonat et al.\textsuperscript{37} presented a rigorous proof for using the Bloch wave function in the microscale stability analysis of general three-dimensional (3D) periodic solids of infinite size, and established the connection between the instabilities at micro and macro scales. That is, the buckling mode of infinite wavelength at microscale can be equivalently detected as a loss of rank-1 convexity of the homogenized tangent moduli at macroscale. Moreover, the homogenization results are only valid before the bifurcation occurs and these results lose their validity after the onset of bifurcation. Thus, the determination of the onset of such micro/macro instabilities is critical for understanding the behavior of nonlinear periodic materials (metamaterials). To investigate such phenomena, the Bloch wave analysis has been used in the past studies for understanding the stability behavior of various periodic composites.\textsuperscript{38–42} Some of the microscale buckling modes have been successfully captured in experimental studies.\textsuperscript{43,44} In addition to the Bloch wave method, other methods, such as stability analysis on RVEs of increasing size,\textsuperscript{45,46} the block-diagonalization method of group-theoretic bifurcation theory,\textsuperscript{47} and others\textsuperscript{48,49} have also been pursued for this purpose. Although these efforts represent important contributions toward understanding the behavior of nonlinear periodic materials, there is a lack of a general clear and consistent computational frameworks that can be effectively used toward this end.

The main contribution of this work is to provide a consistent computational framework for both finite strain homogenization and multiscale stability analyses of periodic microstructures of rate-independent solids with implementation...
details. While some of the methods were presented by the authors in the context of topology optimization and isogeometric analysis,\textsuperscript{2,50,51} in this study an effort is made to unify the presentation and to further develop and clarify the corresponding computational schemes. Specifically, the homogenization is formulated based on the principle of multiscale virtual power with Lagrange multipliers for periodic boundary enforcement. A consistent derivation is presented for both strain and stress driven cases based on a priori discretized microstructure. The implementation details of the Bloch wave analysis are presented, which include the selection of the wave vector space and the retrieval of the real-valued buckling mode from the complex-valued Bloch wave representation. Three different treatments for the resulted constrained eigenvalue problems—two condensation methods and a null-space projection method—are detailed. The implementation of the multiscale homogenization and stability analyses is verified through numerical examples with both hyperelastic and elastoplastic periodic materials. Different choices of RVE are discussed and it is shown that both homogenization and stability results are consistent, irrespective of the choice of the RVE. Depending on the considered material microstructure and loading conditions, different types of buckling modes are observed including short-wavelength buckling with wavelength across one or multiple unit cells and long-wavelength buckling of infinite wavelength with respect to the unit cell size. Furthermore, different types of bifurcation points—simple, double, and triple—are also shown in different test cases. It should be noted that the presented framework is based on the assumption of scale separation, that is, $L \gg l$ with $L$ and $l$ the characteristic lengths of the macro and micro scales, respectively. The scale effect on the homogenization and stability is out of the scope of this study. Interested readers are referred to References 27 and 52,53 for further details on these topics.

The rest of this article is organized as follows: In Section 2, a detailed formulation of the finite strain homogenization is presented. Part of the framework was presented earlier by the authors in a topology optimization context\textsuperscript{2,51} and is further clarified and expanded here for stress-driven homogenization. In Section 3, numerical examples are carried out that verify the homogenization framework in the current context. Important theoretical aspects and implementation details of the Bloch wave method in microscale stability analysis and the macroscale rank-1 convexity analysis are presented in Section 4. Various numerical examples that verify the stability analysis implementation and illustrate different types of microscale instability are given in Section 5. Finally, remarks and conclusions are given in Section 6.

2 FINITE DEFORMATION HOMOGENIZATION

Consider a material as shown in Figure 1, which is made up of periodic microstructure. The periodic microstructure can be characterized by a representative volume element (RVE). The RVE can include one or more fundamental periodic cells (i.e., unit cells). To fulfill the scale separation assumptions, the characteristic length of RVE should be much smaller than the dimensions of the macroscale continuum material.\textsuperscript{33} In the initial configuration, the general shape of the periodic RVE in two-dimensional (2D) is a parallelogram, see Figure 1 where $\Omega_0^\mu$ consists of a solid part $B_0$ and void part $H_0$, that is, $\Omega_0^\mu = B_0 \cup H_0$.

Upon the application of boundary and loading conditions, the macroscale continuum undergoes a nonlinear deformation $\overline{\varphi}$ which maps the continuum from the initial configuration $\Omega_0$ to the current configuration $\Omega$, that is, $\overline{x}(t) = \overline{\varphi}({\overline{X}}, t)$ at $\overline{X} \in \Omega_0$, $t \in \mathbb{R}^+$. Correspondingly, the RVE at material point $\overline{X}$ deforms from its initial configuration $\Omega_0^\mu$ to its current configuration $\Omega_t^\mu$ through a nonlinear mapping $\varphi$, that is, $x(t) = \varphi(X, t)$ at $X \in \Omega_0^\mu$, $t \in \mathbb{R}^+$. Here an overbar is used to denote variables at macroscale, for example, $\overline{x}$ and $\overline{X}$ are the position vectors of a material point in the initial and current configurations, respectively, at macroscale, while $X$ and $x$ are position vectors of a material point in the initial and current configurations, respectively, at microscale. An implicit assumption on the deformation is that the periodicity of the microstructure remains unchanged from the initial to the current configurations. Hence, the deformed RVE still serves as a periodic cell in the deformed microstructure, and can be homogenized for estimating the macrosopic material properties.

In the deformation-driven homogenization framework, deformation of the microstructure located at $\overline{X}$ is driven by a local deformation gradient $\overline{F}(\overline{X}, t) = I + \nabla_{\overline{X}} \overline{u}$ where $\overline{u}$ is the macroscopic displacement field satisfying $\overline{x}(t) = \overline{x} + \overline{u}(t)$ and $\nabla_{\overline{X}}$ represents the gradient operator w.r.t. the macroscale coordinates $\overline{X}$. In this study, the macroscopic deformation $\overline{F}(\overline{X}, t)$ is prescribed at certain fixed $\overline{X} \in \Omega_0$, without referring to any specific macroproblem. The macroscopic material properties, that is, homogenized/macroscopic stress and tangent moduli, are then evaluated under this deformation mode. Thus, the explicit dependence on $\overline{X}$ is omitted in further discussions.

The microscopic displacement field $u(X, t)$ over the RVE domain $\Omega_0^\mu$ is assumed to be driven by a prescribed macroscopic deformation $\overline{F}(t)$, that is,
\[ u(X, t) = (\bar{F}(t) - I)X + \tilde{u}(X, t), \]

where \( \tilde{u}(X, t) \) is the displacement fluctuation field. Correspondingly, the microscopic deformation gradient reads

\[ F(X, t) = \bar{F}(t) + \nabla_X \tilde{u}(X, t), \]

where \( \nabla_X \) denotes the gradient operator w.r.t. the microscale coordinates \( X \). Following Reference 25, the microscale displacement field has to satisfy the kinematical admissibility constraints, which are postulated as

\[ \int_{\Omega_0} u(X, t) dV = 0 \quad \text{and} \quad \bar{F}(t) = I + \frac{1}{V} \int_{\partial \Omega_0^\mu} u(X, t) \otimes N(X) dS \]

in which \( V \) is the volume of the domain \( \Omega_0^\mu \) and \( N \) is the unit normal vector on the boundary \( \partial \Omega_0^\mu \). Applying divergence theorem to Equation (3)_2 gives

\[ \bar{F}(t) = I + \frac{1}{V} \int_{B_0} \nabla_X u(X, t) dV - \frac{1}{V} \int_{\partial B_0} u(X, t) \otimes N(X) dS \]

which shows that in general the macroscopic deformation gradient \( \bar{F}(t) \) is not equal to the volume average of the microscopic deformation gradient \( F(X, t) \) due to the presence of the voids,\(^21\) where note that \( \partial B_0 = \partial \Omega_0^\mu \cup \partial \mathcal{H}_0 \) with \( \partial(\square) \) representing the boundary of \( \square \). Again using the divergence theorem, it can be shown that Equations (3)_1 and (3)_2 are equivalent to

\[ \int_{B_0} \tilde{u}(X, t) dV = 0 \quad \text{and} \quad \int_{\partial \Omega_0^\mu} \tilde{u}(X, t) \otimes N(X) dS = 0, \]

where it is assumed that the coordinate system on microscale is chosen such that \( \int_{B_0} XDV = 0 \). It can be seen that the constraint in Equation (3)_1 is equivalent to removing rigid-body translation, while the constraint in Equation (3)_2 implicitly removes rigid-body rotation. Thus, the kinematically admissible displacement fluctuation field \( \tilde{u}(X, t) \) is defined in a functional space \( \mathcal{V}_{\text{min}} \).
where $H^1(B_0) = \{ v | v_i \in L^2(B_0), \partial v_i / \partial X_j \in L^2(B_0), i, j = 1, 2, \ldots, d \}$ and $L^2(B_0)$ represents the space of square-integrable functions defined on $B_0$ and $d$ is the number of space dimensions. The subscript $\min$ means that this set of constraints is the minimal set required for kinematical admissibility. As shown in Appendix A, this set of constraints corresponds to the constant traction boundary conditions, that is,

$$t_0(X, t) = \overline{P}(t).N(X) \text{ on } \partial \Omega_0^\mu,$$

where $t_0(X, t) = \overline{P}(X, t).N(X)$ represents the first Piola–Kirchhoff (nominal) traction acting on the reference surface with normal $N(X)$; $P(X, t)$ denotes the first Piola–Kirchhoff (PK) stress on the microscale at position $X$ at time instant $t$, while $\overline{P}(t)$ represents the macroscopic/homogenized first PK stress at time $t$ (see Equation 13). Additional constraints can be introduced in a consistent way that may lead to periodic boundary conditions or linear displacement boundary conditions.

### Periodic boundary condition

For RVE, the boundary can be divided into a pair of negative and positive sides, denoting as $\partial \Omega_0^-\mu$ and $\partial \Omega_0^+\mu$, respectively, see Figure 2 where points on the positive side can be reached by translating the corresponding points on the negative side using a periodic lattice vector $a_1$ or $a_2$ or $\pm(a_1 \pm a_2)$. For the periodic boundary conditions, the displacement fluctuations on the negative side equal the corresponding ones on the positive side, that is,

$$\tilde{u}^+ = \tilde{u}^- \text{ on } \partial \Omega_0^\mu$$

which can be proved to automatically satisfy the constraints in Equations (3)$_2$ or (5)$_2$. As a result, the kinematically admissible displacement fluctuation field considering periodic boundary condition is defined in a functional space $Y_p$

$$Y_p = \left\{ \tilde{u}(X, t)|\tilde{u}(X, t) \in H^1(B_0), t \in \mathbb{R}^+, \int_{B_0} \tilde{u}(X, t) dV = 0, \tilde{u}^+(t) = \tilde{u}^-(t) \text{ on } \partial \Omega_0^\mu \right\}.$$

### Linear displacement boundary condition

The linear displacement boundary condition requires zero displacement fluctuations on the boundaries, that is,

$$\tilde{u} = 0 \text{ on } \partial \Omega_0^\mu$$

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**Figure 2** Geometries and partitioning of boundary nodes of discretized microstructures of RVE (blue color denotes the negative nodes and red color denotes the positive nodes). RVE, representative volume element.
which satisfies the constraints in Equation (8) and also constraints in Equations (3) or (5). The corresponding functional space \( V_l \) for the kinematically admissible displacement fluctuation field reads

\[
V_l = \{ \tilde{\mathbf{u}}(\mathbf{X}, t) | \tilde{\mathbf{u}}(\mathbf{X}, t) \in H^1(B_0), t \in \mathbb{R}^+ \},
\]

and \( \tilde{\mathbf{u}}(t) = 0 \) on \( \partial \Omega^0 \). (11)

The transition between the micro and macro scales is governed by the principle of multiscale virtual power, \(^{25}\) which is expressed as,

\[
\bar{\mathbf{P}} : \delta \bar{\mathbf{F}} = \frac{1}{V} \int_{B_0} \mathbf{P} : \delta \mathbf{F} \, dV \quad \forall \delta \bar{\mathbf{F}} \in \text{Lin}, \ \delta \tilde{\mathbf{u}} \in \mathcal{V},
\]

(12)

where \( \bar{\mathbf{P}} \) and \( \mathbf{P} \) are the first PK stress tensors on macro and micro scales, respectively, and the space of the virtual fluctuation field \( \delta \tilde{\mathbf{u}} \) is identical to that of the fluctuation field \( \tilde{\mathbf{u}} \), \( \mathcal{V} \), which can be \( \mathcal{V}_{\text{min}}, \mathcal{V}_p \), or \( \mathcal{V}_l \). Equation (12) can be seen as the variational form of the Hill–Mandel condition \(^{14,24}\) that states the equivalence of the incremental virtual work between the micro and macro scales.

The stress homogenization relation

\[
\bar{\mathbf{P}} = \frac{1}{V} \int_{B_0} \mathbf{P} \, dV = \frac{1}{V} \int_{\partial B_0} \mathbf{t}_0 \otimes \mathbf{x} \, dS = \frac{1}{V} \int_{\partial \Omega^0} \mathbf{t}_0 \otimes \mathbf{x} \, dS \quad \text{with} \quad \mathbf{t}_0 = \mathbf{P} \mathbf{N}
\]

(13)

and the microscale equilibrium equation

\[
\int_{B_0} \mathbf{P} : \nabla \delta \tilde{\mathbf{u}} \, dV = 0 \quad \forall \delta \tilde{\mathbf{u}} \in \mathcal{V}
\]

(14)

can be obtained from Equation (12) by choosing \( \delta \tilde{\mathbf{u}} = 0 \) and \( \delta \bar{\mathbf{F}} = 0 \), respectively. Here, the second equality in Equation (13) can be proved using divergence theorem and the fact that \( \nabla \mathbf{x} \mathbf{P} = 0 \), while the third equality is due to the traction-free void boundaries, that is, \( \mathbf{t}_0 = 0 \) on \( \partial H_0 \).

2.1 Deformation driven homogenization

In this section, a deformation-driven homogenization formulation for computing the homogenized stresses and tangent moduli of a priori discretized microstructure is presented. For ease of the derivation of homogenized quantities, the Lagrange multiplier is adopted to enforce the boundary condition. Other methods such as the condensation method can also be used. \(^{33}\) As shown in Figure 1 that the geometry of RVE must satisfy certain constraints to be compatible with periodicity. For instance, the most general RVE shape for 2D problems is the parallelogram (Figures 1 or 2(A)), and square or rectangular shapes are special cases of a parallelogram. The hexagonal unit cell (Figure 2(B)) can also be equivalently recast into a parallelogram. In this study, 2D problems (plane strain) are considered in the numerical implementations, however, all the presented methods can be canonically extended to 3D cases. Since the underlying microstructure of the periodic materials is always assumed to be periodic with repeating unit cells (Figure 1), the periodic boundary conditions are chosen, \(^{37}\) that is, \( \mathcal{V} = \mathcal{V}_p \) in Equation (12).

Consider now for a given discretized RVE (Figure 2), the constraints in Equation (8) are discretized as

\[
\bar{\mathbf{u}}_q^+ = \bar{\mathbf{u}}_q, \quad q = 1, 2, \ldots, m,
\]

(15)

where \( m \) pairs of nodes lying on the negative and positive boundary sides are identified. For example, \( m = 17 \) for the parallelogram RVE in Figure 2(A) including 14 pairs on the inner positive/negative sides and three pairs at the corners (see Remarks in Section 2.1.1). The rigid-body translation constraint (Equation (5)_1) can be equivalently replaced by fixing one arbitrary point, for example, \( \bar{\mathbf{u}}_o = 0 \) in \( B_0 \). Thus, the discretized functional space \( \mathcal{V}^h \) is defined by

\[
\mathcal{V}^h = \{ \tilde{\mathbf{u}}(\mathbf{X}, t) | \tilde{\mathbf{u}}(\mathbf{X}, t) \in H^1(B_0), t \in \mathbb{R}^+ \}, \ \tilde{\mathbf{u}}_o = 0, \ \bar{\mathbf{u}}_q^+ = \bar{\mathbf{u}}_q^-(q = 1, 2, \ldots, m) \}.
\]

(16)
2.1.1 Principle of multiscale virtual power with Lagrange multiplier—discrete form

Using the Lagrange multipliers to enforce the constraints in Equation (16), the discretized version of the principle of multiscale virtual power is expressed as

$$-V(\mathbf{F} : \delta \mathbf{F}) + \int_{B_0} P : \delta P dV - \delta \lambda^T \mathbf{u}_0 - \lambda^T \delta \mathbf{u}_0 - \sum_{q=1}^{m} \delta \mu_q^T [\mathbf{u}_q^+ - \mathbf{u}_q^- - (\mathbf{F} - I) \mathbf{L}_q]$$

$$- \sum_{q=1}^{m} \mu_q^+ [\delta \mathbf{u}_q^+ - \delta \mathbf{u}_q^- - \delta \mathbf{F} \mathbf{L}_q] = 0 \forall \delta \mathbf{F} \in \text{Lin}, \quad \delta \mathbf{u} \in H^1(B_0), \quad \delta \lambda, \quad \delta \mu,$$

(17)

where $\lambda$ and $\mu = [\mu_1, \ldots, \mu_m]^T$ are the Lagrange multipliers, and the constraints are restated in terms of the displacement field $\mathbf{u}(\mathbf{X}, t)$ instead of fluctuation field $\tilde{\mathbf{u}}(\mathbf{X}, t)$. Note that $\mathbf{u}_o(t) = 0$ is equivalent to $\tilde{\mathbf{u}}_o(t) = 0$ in the sense of removing rigid-body translations. The vector $\mathbf{L}_q$ in Equation (17) represents the translation vector that satisfies $\mathbf{X}_q^+ = \mathbf{X}_q^- + \mathbf{L}_q$ where $\mathbf{X}_q^+$ and $\mathbf{X}_q^-$ are the coordinates of the nodes on a pair of positive and negative sides, see Figure 2.

Remarks. : For the $m$ pairs of periodic boundary condition constraints, the inner nodes on each positive and negative sides can be easily identified and related through the periodic translation vectors. For the end nodes on the sides, that is, corner nodes, special care is needed for identifying sufficient and necessary constraints that represent the periodic boundary conditions. For example, Figure 3 shows the parallelogram and hexagon cases where only the periodic constraints that are related to the corner nodes are demonstrated. As can be seen, after the removal of the repeated constraints, three constraints are needed for parallelogram RVE that identify three pairs of negative and positive corner nodes, while four constraints are needed for hexagon RVE that identify four pairs of negative and positive corner nodes. It should be noted that the constraints listed in Figure 3 can be restated in multiple ways as long as the constraints are linearly independent, for example, the second equation in Figure 3(A) can be restated as $\mathbf{u}_3 = \mathbf{u}_1 + \nabla_X \tilde{\mathbf{u}}(\mathbf{a}_1 + \mathbf{a}_2)$.

2.1.2 Interpretation of Lagrange multipliers

The Lagrange multipliers $\lambda$ and $\mu$ can be interpreted as discrete nodal forces on the boundary. For instance, assuming $\delta \mathbf{F} = 0$, $\delta \lambda = 0$, and $\delta \mu = 0$ and $\delta \mathbf{u} = c_0$ (with $c_0$ constant in $B_0$) in Equation (17) gives $\lambda^T c_0 = 0$. Therefore,

(A) Periodic boundary conditions for corner nodes

$$\begin{align*}
\mathbf{u}_2 &= \mathbf{u}_1 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_1 \\
\mathbf{u}_3 &= \mathbf{u}_4 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_3 \\
\mathbf{u}_4 &= \mathbf{u}_1 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_2 \\
\mathbf{u}_3 &= \mathbf{u}_2 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_2 \quad \leftarrow \text{(repeated, remove!)}
\end{align*}$$

Parallelgram unit cell

(B) Periodic boundary conditions for corner nodes

$$\begin{align*}
\mathbf{u}_5 &= \mathbf{u}_1 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{H} \\
\mathbf{u}_4 &= \mathbf{u}_5 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{H} \quad \leftarrow \text{(repeated, remove!)} \\
\mathbf{u}_3 &= \mathbf{u}_1 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_3 \\
\mathbf{u}_4 &= \mathbf{u}_3 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_3 \\
\mathbf{u}_2 &= \mathbf{u}_4 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_2 \\
\mathbf{u}_3 &= \mathbf{u}_5 + \nabla_X \tilde{\mathbf{u}} \cdot \mathbf{a}_2 \quad \leftarrow \text{(repeated, remove!)}
\end{align*}$$

Hexagon unit cell

F I G U R E 3 Periodic boundary conditions for corner nodes ($\mathbf{H} = \mathbf{a}_1 - \mathbf{a}_2$ in (B))
\[ \lambda = 0 \] (18)

has to be satisfied, which means that for a self-equilibrated system, fixing one arbitrary point for removing rigid-body translation does not create any reaction forces. Next, taking \( \delta \bar{F} = 0, \delta \lambda = 0, \) and \( \delta \mu = 0 \) with \( \delta \mathbf{u}(\mathbf{X}) = \mathbf{A}_0 \mathbf{X} \) in \( B_0 \) where \( \mathbf{A}_0 \in \text{Lin} \) (a constant second-order tensor) in Equation (17), it can be shown that

\[
\left( \int_{B_0} \mathbf{P} dV - \sum_{q=1}^{m} \mu_q \otimes \mathbf{L}_q \right) : \mathbf{A}_0 = 0 \quad \forall \mathbf{A}_0 \in \text{Lin},
\]

(19)

where \( \mu_q \) and \( \mathbf{L}_q \) \((q = 1, \ldots, m)\) are both vectors (or first-order tensors) while \( \mathbf{P} \) and \( \mathbf{A}_0 \) are second-order tensors. Since \( \mathbf{A}_0 \) can be chosen arbitrarily, it follows from Equations (13) and (19) that

\[
\overline{\mathbf{P}} = \frac{1}{V} \int_{B_0} \mathbf{P} dV = \frac{1}{V} \sum_{q=1}^{m} \mu_q \otimes \mathbf{L}_q
\]

(20)

which when combined with Equation (13), shows that \( \mu_q \) represents the traction force at node \( q \). Therefore, it can be seen that the homogenized stress can be computed from the Lagrange multipliers \( \mu \).

2.1.3 Finite element formulation

Considering the unknown variables to be solved as \( \mathbf{u}, \lambda, \) and \( \mu, \) the resulting set of nonlinear constrained equilibrium equations, from Equation (17), can be written as

\[
\mathbf{R}(\mathbf{u}, \lambda, \mu) = \begin{bmatrix} \mathbf{R}_1(\mathbf{u}, \lambda, \mu) \\ \mathbf{R}_2(\mathbf{u}) \\ \mathbf{R}_3(\mathbf{u}) \end{bmatrix} = \begin{bmatrix} \mathbf{F}_{\text{int}}(\mathbf{u}) - \mathbf{A}_1^T \lambda - \mathbf{A}_2^T \mu \\ - \mathbf{A}_1 \mathbf{u} \\ - \mathbf{A}_2 \mathbf{u} \end{bmatrix} + \begin{bmatrix} 0 \\ \mathbf{h} \end{bmatrix} = \mathbf{0},
\]

(21)

where \( \mathbf{F}_{\text{int}} \) represents the global internal force vector defined by

\[
\mathbf{F}_{\text{int}}(\mathbf{u}) = \sum_{e=1}^{n_{\text{ele}}} \mathbf{F}_{\text{int}}^e = \sum_{e=1}^{n_{\text{ele}}} \int_{\Omega^e} \mathbf{B}^T \mathbf{P} dV,
\]

(22)

where \( \mathbf{B} \) is the shape function derivative matrix, \( \Omega^e \) represents the \( e \)th element integration domain satisfying \( B_0 = \bigcup_{e=1}^{n_{\text{ele}}} \Omega^e \) and \( n_{\text{ele}} \) are the total number of elements in the RVE.

The matrices \( \mathbf{A}_1 \) and \( \mathbf{A}_2 \), and vector \( \mathbf{h} \) are constructed such that

\[
\mathbf{u}_0 = \mathbf{A}_1 \mathbf{u},
\]

\[
\mathbf{u}^+ - \mathbf{u}^- = \mathbf{A}_2 \mathbf{u},
\]

\[
\mathbf{h} = \begin{bmatrix} \mathbf{(F} - \mathbf{I}).\mathbf{L}_1 \\ \vdots \\ \mathbf{(F} - \mathbf{I}).\mathbf{L}_m \end{bmatrix} = [\mathbf{L}_M](\mathbf{[F]} - [\mathbf{I}]) = \begin{bmatrix} \mathbf{X}_1 & 0 & \mathbf{Y}_1 & 0 \\ 0 & \mathbf{X}_1 & 0 & \mathbf{Y}_1 \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{X}_m & 0 & \mathbf{Y}_m & 0 \\ 0 & \mathbf{X}_m & 0 & \mathbf{Y}_m \end{bmatrix}_{2m \times 4} \begin{bmatrix} \mathbf{F}_{11} \\ \mathbf{F}_{21} \\ \mathbf{F}_{12} \\ \mathbf{F}_{22} \end{bmatrix}_{4 \times 1} + \begin{bmatrix} 1 \\ 0 \end{bmatrix}_{2 \times 1},
\]

(23)

where \( \mathbf{u} \) is the global nodal displacement vector, \( \mathbf{u}^+ = [\mathbf{u}^+_1, \ldots, \mathbf{u}^+_m]^T \) and \( \mathbf{u}^- = [\mathbf{u}^-_1, \ldots, \mathbf{u}^-_m]^T \) includes nodal displacements defined on the positive and negative boundary sides, respectively. \( \mathbf{L}_q = [\mathbf{X}_q, \mathbf{Y}_q]^T \) is the translational vector from the \( q \)th node on the negative side to the \( q \)th node on the positive side. The expression of \( \mathbf{h} \) vector is written for 2D case in Equation (23).
The nonlinear system in Equation (21) is solved using the Newton–Raphson (NR) method and the Jacobian matrix, which is needed for NR solver, can be calculated as

\[ [J_T] = \begin{bmatrix}
\frac{\partial R_1}{\partial u} & \frac{\partial R_1}{\partial \lambda} & \frac{\partial R_1}{\partial \mu} \\
\frac{\partial R_2}{\partial u} & \frac{\partial R_2}{\partial \lambda} & \frac{\partial R_2}{\partial \mu} \\
\frac{\partial R_3}{\partial u} & \frac{\partial R_3}{\partial \lambda} & \frac{\partial R_3}{\partial \mu}
\end{bmatrix} = \begin{bmatrix}
K_T & -A_1^T & -A_2^T \\
-A_1 & 0 & 0 \\
-A_2 & 0 & 0
\end{bmatrix}, \tag{24}\]

where the term \( K_T \) is the tangent structural stiffness matrix calculated by

\[ K_T = \frac{\partial F_{int}}{\partial u} = \sum_{i=1}^{N_n} k_i^T \] with \( k_i = \int_{\Omega} B^T[A]B \, dV \) and \( A = \frac{\partial P}{\partial F} \) \tag{25}\]

in which the tangent moduli \( A \) is obtained from material subroutine. Here, the bracket outside \( A \) means that it is arranged in a matrix form, for example, \( 9 \times 9 \) matrix in 3D case and \( 4 \times 4 \) matrix for 2D plane strain case.

### 2.1.4 Homogenized stress and tangent moduli

Using Equation (20) and the definition of matrix \( [L_M] \) given in Equation (23), the homogenized stress \( \overline{P} \) is computed as

\[ \overline{P} = \frac{1}{V} [L_M]^T \mu. \tag{26}\]

where the bracket outside \( \overline{P} \) means that it is arranged in a \( 4 \times 1 \) vector form (2D), similarly as \( [F] \) used in Equation (23).

The fourth-order tensor homogenized tangent moduli \( \overline{A} \) is defined by

\[ \overline{A} = \frac{\partial \overline{P}}{\partial \overline{F}} \tag{27}\]

and can be rephrased in a matrix form as \( \overline{[A]} = \partial [\overline{P}] / \partial [\overline{F}] \), which is of size \( 4 \times 4 \) for 2D case. From Equation (26), it is clear that \( \overline{[A]} \) is determined by the derivative of Lagrange multiplier \( \mu \) with respect to \( \overline{F} \). To this end, the set of global equilibrium equation (Equation 21) is perturbed at the equilibrium state by a perturbation \( \Delta \overline{F} \), that is,

\[ \begin{bmatrix}
K_T & -A_1^T & -A_2^T \\
-A_1 & 0 & 0 \\
-A_2 & 0 & 0
\end{bmatrix} \begin{bmatrix}
\Delta u \\
\Delta \lambda \\
\Delta \mu
\end{bmatrix} + \begin{bmatrix}
0 \\
0 \\
L_M
\end{bmatrix} = [\Delta \overline{F}] = 0 \tag{28}\]

which results in

\[ \begin{bmatrix}
\Delta u \\
\Delta \lambda \\
\Delta \mu
\end{bmatrix} = -[J_T]^{-1} \begin{bmatrix}
0 \\
0 \\
L_M
\end{bmatrix} [\Delta \overline{F}] \tag{29}\]

Combining Equation (27) with Equations (26) and (29), it can be shown that

\[ \overline{[A]} = -\frac{1}{V} [\hat{L}_M]^T [J_T]^{-1} [\hat{L}_M] \tag{30} \]

where the matrix \( [\hat{L}_M] \) is of size \( (N + 2 + 2m) \times 4 \) for a 2D case and is defined by

\[ [\hat{L}_M] = \begin{bmatrix}
0_{Nx4} \\
0_{2x4} \\
[L_M]_{2m4}
\end{bmatrix} \tag{31}\]

where \( N \) is the number of total DOFs in the displacement field, that is, the size of \( u \) vector.
2.2 Stress driven homogenization

In the stress driven homogenization, the macro Kirchhoff stress tensor \( \bar{\tau} = \bar{P} \bar{F}^T \) is prescribed and drives the homogenization analysis. Due to the principle of conservation of angular momentum, the macro Kirchhoff stress tensor is symmetric, that is, \( \bar{\tau} = \bar{\tau}^T \). In order to use the deformation driven homogenization analysis. Due to the principle of conservation of angular momentum, the macro Kirchhoff stress tensor is symmetric, that is, \( \bar{\tau} = \bar{\tau}^T \). In order to use the deformation driven homogenization framework presented in Section 2.1, the deformation gradient \( \bar{F} \) has to be solved for the prescribed \( \bar{\tau} \). Without loss of generality, the macroscopic rigid-body rotation is ignored, that is, \( \bar{R} = I \) or \( \bar{U} = \vec{U} \), and thus \( \bar{F} \) is symmetric. Hence, the problem is now rephrased as determining \( \bar{F}_{11}, \bar{F}_{22}, \) and \( \bar{F}_{12} = -\bar{F}_{21} \) for a given, \( \bar{\tau} \), that is, \( \bar{\tau}_{11}, \bar{\tau}_{22}, \) and \( \bar{\tau}_{12} = -\bar{\tau}_{21} \). It is noted that the macro Kirchhoff stress tensor \( \bar{\tau} \) is used as the applied macroscopic stress instead of the macro Cauchy stress as they differ only by a scalar \( \bar{J} = \det{\bar{F}} \), which does not change the principal stress directions, and the focus in this study is on the multiscale stabilities under different loading paths in the principal stress space. To this end, suppose the principal macrostresses \( \bar{\tau}_a \) (\( a = 1, 2 \) for 2D case) are at a fixed angle \( \theta \) with respect to the standard Euclidean bases \( \{\vec{e}_a\} \), that is,

\[
\bar{\tau} = \bar{Q} \bar{\tau}' \bar{Q}^T \quad \text{with} \quad Q(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \quad \text{and} \quad \bar{\tau}' = \begin{bmatrix} \tau_{11}' & \tau_{12}' \\ \tau_{21}' & \tau_{22}' \end{bmatrix} = \begin{bmatrix} \tau_1 & 0 \\ 0 & \tau_2 \end{bmatrix}
\]  

(32)

with \( \bar{Q} \) the bases transformation matrix, or written equivalently in matrix-vector form as

\[
[\bar{\tau}] = [Q][\bar{\tau}'] \quad \text{or} \quad [\bar{\tau}'] = [Q]^T[\bar{\tau}]
\]  

(33)

where \([\bar{\tau}] = [\bar{\tau}_{11} \quad \bar{\tau}_{21} \quad \bar{\tau}_{12} \quad \bar{\tau}_{22}]^T \) and \([\bar{\tau}'] = [\bar{\tau}_{11}' \quad \bar{\tau}_{21}' \quad \bar{\tau}_{12}' \quad \bar{\tau}_{22}']^T (= [\tau_1 \quad 0 \quad 0 \quad \tau_2]^T) \) are the vector forms of \( \bar{\tau} \) and \( \bar{\tau}' \), respectively, and

\[
[Q] = \begin{bmatrix}
\cos^2 \theta & -\sin \theta \cos \theta & -\sin \theta \cos \theta & \sin^2 \theta \\
\sin \theta \cos \theta & \cos^2 \theta & -\sin^2 \theta & -\sin \theta \cos \theta \\
\sin \theta \cos \theta & -\sin^2 \theta & \cos^2 \theta & -\sin \theta \cos \theta \\
\sin^2 \theta & \sin \theta \cos \theta & \sin \theta \cos \theta & \cos^2 \theta
\end{bmatrix}.
\]  

(34)

Without loss of generality, the principal stresses \( \bar{\tau}_a \) are parameterized as

\[
\bar{\tau}_1 = -\lambda \cos \phi \quad \text{and} \quad \bar{\tau}_2 = -\lambda \sin \phi,
\]  

(35)

where \( \lambda \) is the amplitude of load (positive in compression) and \( \phi \) controls the ratio of the macro principal stresses. As a result, the stress state \( \bar{\tau} \) is fully described by three parameters \( \lambda, \phi, \) and \( \theta \). Thus, the pure stress driven homogenization can be formulated as two nested loops, with inner loop formulated as deformation driven homogenization and outer loop formulated as a system of nonlinear equations that is solved for deformation gradient \( \bar{F} \) for a prescribed stress tensor \( \bar{\tau} \). The nonlinear equations for the outer loop can be expressed as

\[
R_{\tau} = \begin{bmatrix}
\bar{\tau}_{11} & \bar{\tau}_{12} & \bar{\tau}_{22} \\
\bar{\tau}_{21} & \bar{\tau}_{22} & \bar{\tau}_{21} \\
\bar{\tau}_{22} & \bar{\tau}_{11} & \bar{\tau}_{22}
\end{bmatrix} - \begin{bmatrix} \lambda \cos \phi \\ 0 \\ \lambda \sin \phi \end{bmatrix} = \mathbf{0},
\]  

(36)

where \( \bar{\tau}_{ij} \) are computed from Equation (33)\(_2\). The NR method is used to solve above nonlinear equations for \( \bar{F}_{11}, \bar{F}_{22}, \) and \( \bar{F}_{12} (= \bar{F}_{21}) \). To calculate the Jacobian matrix, it is easy to denote

\[
\begin{bmatrix}
\bar{\tau}_{11} \\
\bar{\tau}_{12} \\
\bar{\tau}_{22}
\end{bmatrix} = \begin{bmatrix}
\cos^2 \theta & -\sin \theta \cos \theta & -\sin \theta \cos \theta & \sin^2 \theta \\
\sin \theta \cos \theta & -\sin^2 \theta & \cos^2 \theta & -\sin \theta \cos \theta \\
\sin^2 \theta & \sin \theta \cos \theta & \sin \theta \cos \theta & \cos^2 \theta
\end{bmatrix} [\bar{\tau}] = [T][\bar{\tau}],
\]  

(37)
where matrix $[T]$ is $[Q]^T$ with the second row being removed. Next, due to the symmetry assumption, the deformation gradient is expressed as

$$[\hat{F}] = \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} = [I_3][\hat{F}], \quad (38)$$

where $[\hat{F}]$ are the unknown variables that are to be solved. Moreover, from $\tau = \hat{P}F^T$, it can be shown that

$$[\hat{F}] = [\hat{F}][\hat{P}] = [\hat{F}]$$

(39)

with

$$[\hat{P}] = \begin{bmatrix} P_{11} & 0 & P_{12} & 0 \\ 0 & P_{11} & 0 & P_{12} \\ P_{21} & 0 & P_{22} & 0 \\ 0 & P_{21} & 0 & P_{22} \end{bmatrix} \quad \text{and} \quad [\hat{F}] = \begin{bmatrix} F_{11} & 0 & F_{12} & 0 \\ F_{21} & 0 & F_{22} & 0 \\ 0 & F_{11} & 0 & F_{12} \\ 0 & F_{21} & 0 & F_{22} \end{bmatrix}. \quad (40)$$

With the above notations, the Jacobian matrix $[J_{\tau}] = \partial R_{\tau} / \partial \hat{F}$ can be obtained as

$$[J_{\tau}] = [T] \frac{\partial [\tau]}{\partial [\hat{F}]} [I_{43}] \quad (41)$$

with

$$\frac{\partial [\tau]}{\partial [\hat{F}]} = [\hat{P}] + [\hat{F}]A. \quad (42)$$

which is derived from Equation (39).

### 3 | NUMERICAL VERIFICATION—HOMOGENIZATION ANALYSIS

This section numerically investigates the sufficiency of using one unit cell as RVE for homogenization analysis as well as the equivalency of different choices of unit cells from the same periodic material. Both hyperelastic and elastoplastic constituent phases are considered. Specifically, the hyperelastic material phase is modeled by the regularized (compressible) neo-Hookean hyperelastic model for which the free energy is expressed as

$$\psi(C) = \frac{1}{2} \kappa (J - 1)^2 + \frac{\mu}{2} (I_1 - 3), \quad (43)$$

where $C$ is the right Cauchy–Green tensor and $I_1$ is the first invariant of $\bar{C}$, that is, $I_1 = \text{tr} \bar{C}$ with $\bar{C} = J^{-2/3}C$ and $J$ the determinant of the deformation gradient. $\kappa$ and $\mu$ are bulk and shear modulus of the material. The elastoplastic material phase is modeled by a finite strain $J_2$ plasticity and the model details are provided in Appendix B. All the computations in this study are carried out using an in-house Matlab-based finite element library CPSSL-FEA developed at the University of Notre Dame.

#### 3.1 | Finite elastic deformations of a periodic material

The first example examines a hyperelastic periodic material that represents path-independent material cases. The periodic material (Figure 4) consists of soft matrix and hard circular inclusions with diameter $d = 0.4$, both of which are modeled
by a regularized neo-Hookean hyperelastic model (Equation (43)). The model parameters are $\kappa_m = 17.5$ and $\mu_m = 8.0$ for matrix and $\kappa_I = 100\kappa_m$ and $\mu_I = 100\mu_m$ for inclusion. The unit cell is of unit side length and unit thickness with inclusion located at either center or position $(-0.2, 0.2)$. It is clear that the two unit cells with circular inclusions located at different positions represent the same periodic material. With four-node (Q4) plane strain FE discretization, the FE meshes of the two unit cells are shown in Figure 4.

The first two tests are carried out on unit cell-1 (Figure 4(A)) to demonstrate that it is sufficient to choose the smallest repeating cell (unit cell) as RVE for homogenization analysis. To this end, both simple tension $\bar{F} = [F_{11} F_{21} F_{12} F_{22}]^T = [1.4 0 0 1]^T$ and simple shear $\bar{F} = [F_{11} F_{21} F_{12} F_{22}]^T = [1 0 0.4 1]^T$ are considered for homogenization analysis on RVE that consists of a different number of unit cell-1. The results are shown in Table 1 and Figure 5 for simple tension and Table 2 and Figure 6 for simple shear. As shown in Tables 1 and 2, the homogenized stress, tangent moduli, and strain energy for RVEs with a different number of unit cell match exactly with each other. Besides, the periodicity with respect to one unit cell of the deformed shape of the material can be seen from Figures 5 to 6.

For periodic material, the size of the smallest repeating cell (unit cell) can be uniquely determined, whereas the choice of unit cell is not unique. For example, the two different unit cells shown in Figure 4(A,B) both represent the same material. Theoretically, the homogenization result should be independent of the choice of the unit cell. To demonstrate this feature, the two different unit cells are analyzed under both simple tension and simple shear. The results are given in Table 3 and Figure 7 for tension while Table 4 and Figure 8 for shear. In this case, the deformed shapes are different due to the different unit cell geometric features as shown in Figures 7 and 8. Moreover, there are also small differences in the calculated homogenized quantities, that is, stress, tangent moduli, and strain energy, as shown in Tables 3 and 4, which can be attributed to different FE meshes and geometric approximations.

### 3.2 Finite elastic-plastic deformation of a periodic material

#### 3.2.1 Invariance w.r.t number/choice of unit cells in RVE

The second example examines finite strain elastoplastic periodic material that represents path-dependent material cases. A similar example has been considered in Reference 54. Both the matrix and inclusion materials are modeled using the

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**FIGURE 4**  FE meshes of two equivalent unit cells of the hyperelastic periodic material

**TABLE 1**  Homogenized quantities from the RVEs consisting of different number of unit cells (unit cell-1) under simple tension

| RVE  | Homogenized first PK stress $[\bar{P}]$ | Homogenized tangent moduli $[\bar{\lambda}]$ | Homogenized stored energy $\bar{\psi}$ |
|------|---------------------------------------|------------------------------------------|---------------------------------|
| 1x1  | 11.6573                               | 26.0259 $-0.0002$ $-0.0003$ 30.2150     |                                               |
| 1x2  | 0                                     | $-0.0002$ 7.5260 $-1.1210$ 0           |                                               |
| 2x1  | 0                                     | $-0.0003$ $-1.1210$ 7.3172 0           |                                               |
| 2x2  | 8.8865                                | 30.2150 0 0 54.4927                     | 2.4347                                       |

Abbreviation: RVE, representative volume element.
finite strain $J_2$ elastoplasticity given in Table B1, where the multiplicative decomposition of the deformation gradient is assumed, that is, $F = F^e F^p$ and the internal variable can be taken as the elastic Finger tensor $b^e$ or equivalently plastic right Cauchy–Green tensor $C^p$ or its inverse $C_p^{-1}$. The matrix material is simulated as elastoplasticity with parameters: $\kappa_m = 17.5$, $\mu_m = 8.0$, $\sigma_f = 0.45$, and $K_p = 0.1$. The inclusion material is simulated as a hyperelastic phase (by choosing $\sigma_f \to \infty$, here $\sigma_f = 10^6$) with parameters: $\kappa_I = 100\kappa_m$ and $\mu_I = 100\mu_m$. Here, the periodic material can be equivalently described by two unit cells, as seen in Figure 9, unit cell-1 and unit cell-2. The FE models of the two unit cells are shown in Figure 10. Both unit cells are of unit side length and unit thickness with the diameter of the hole and inclusions $d = 0.3$. With the origin of a local coordinate system located at the center of the unit cells, for unit cell-1 the inclusions are located at $(-0.2, 0.2)$ and $(-0.2, -0.2)$ and the hole is located at $(0.2, 0)$, while for unit cell-2 the inclusions are at $(0.3, 0.2)$ and $(0.3, -0.2)$ and the hole is at $(-0.3, 0)$.

To address the volumetric locking due to the incompressible plastic flow, the mixed $u/p$ $(9/3)$ element formulation\(^{55}\) is adopted, where the independent pressure field $p$ is taken as $\tau_m$ defined by $\tau_m \overset{\text{def}}{=} (1/3) I : \tau$. The macroscopic deformation gradient loading considers $[\bar{F}] = [\bar{F}_{11} \quad \bar{F}_{21} \quad \bar{F}_{12} \quad \bar{F}_{22}]^T = [1 \quad 0 \quad 0.1 \quad 1]^T$. The sufficiency of RVE consisting of only one unit cell is again examined for representing materials with a path-dependent response. The analyses are carried out with unit cell-1 (Figure 10(A)). The sufficiency is confirmed by the results shown in Table 5.
TABLE 3 Homogenized quantities from the RVEs of different unit cells under simple tension

| RVE               | Homogenized first PK stress $[\vec{P}]$ | Homogenized tangent moduli $[\vec{A}]$ | Homogenized stored energy $\bar{\psi}$ |
|-------------------|-----------------------------------------|-----------------------------------------|-----------------------------------------|
| Unit cell-1       | 11.6573                                 | 26.0259  -0.0002  -0.0003  30.2150             | 2.4347                                  |
|                   | 0                                       | -0.0002  7.5260  -1.1210  0                   |                                         |
|                   | 0                                       | -0.0003  -1.1210  7.3172  0                   |                                         |
|                   | 8.8865                                  | 30.2150  0  0  54.4927                          |                                         |
| Unit cell-2       | 11.6567                                 | 26.0237  0  -0.0001  30.2151             | 2.4346                                  |
|                   | 0                                       | 0  7.5253  -1.1212  0.0001                  |                                         |
|                   | 0                                       | -0.0001  -1.1212  7.3169  0.0002             |                                         |
|                   | 8.8866                                  | 30.2151  0.0001  0.0002  54.4909              |                                         |

Abbreviation: RVE, representative volume element.

and Figure 11. Next, the equivalence of different choices of a unit cell is checked with the two different unit cells shown in Figure 10. The equivalent plastic strain ($\alpha$) distribution on the deformed shapes are shown in Figure 12(A,B), where similar shear band formations can be observed. Their homogenized deformation gradient versus stress curves (note that $\vec{t} = \vec{P} \vec{F}^T$) along the loading are compared in Figure 13, where a close match can be seen. A further comparison is made in Table 6 where the homogenized quantities including first PK stress, tangent moduli and stored elastic strain energy are compared for the two unit cells at the final loading step. Similar to the hyperelastic case in Section 3.1, the small differences herein can be attributed to the different FE mesh and inaccurate geometry modeling.
Table 4Homogenized quantities from the RVEs of different unit cells under simple shear

| RVE        | Homogenized first PK stress $[\bar{P}]$ | Homogenized tangent moduli $[\bar{A}]$ | Homogenized stored energy $\bar{\Psi}$ |
|------------|-----------------------------------------|----------------------------------------|---------------------------------------|
| Unit cell-1| -0.5929 4.0980 3.8687 -0.5731           | 35.1466 -12.9755 11.5362 -2.9184 14.8978 | 0.7710                                 |
| Unit cell-2| -0.5930 4.0976 3.8684 -0.5731           | 35.1459 -12.9752 11.5345 -2.9183 14.8981 | 0.7709                                 |

Abbreviation: RVE, representative volume element.

3.2.2 Invariance w.r.t shape of RVE

To further illustrate the independence of the homogenization analysis results on the different choice of RVEs, consider the periodic material as shown in Figure 14 where the matrix material has the same properties as the elastoplastic matrix material in the previous example (see Figure 9). The elliptical holes are arranged in a periodic lattice as shown in Figure 14. The major and minor axes are $\sqrt{3}/2$ and 0.5 units, respectively, and the major axis is at an angle 30° w.r.t. the horizontal direction. Three different RVEs are chosen, as shown in Figure 14. It should be noted that RVE-1 and RVE-2 both include one unit cell, that is, they are the smallest periodic cells, while RVE-3 is not. The FE meshes of the three RVEs are shown in Figure 15. The deformation again considers simple shear, that is, $\mathbf{F} = \begin{bmatrix} F_{11} & F_{21} & F_{12} \\ F_{21} & F_{22} & F_{12} \end{bmatrix}^T = \begin{bmatrix} 1 & 0 & 0.1 \end{bmatrix}^T$. Figure 16 shows the deformed shape as well as the equivalent plastic strain ($\alpha$) distribution for different RVEs, where...
FIGURE 9 Illustration of two different ways of choosing a unit cell from the same periodic material

FIGURE 10 FE meshes of two different unit cells of the elastoplastic periodic material

TABLE 5 Homogenized quantities from the elastoplastic RVE consisting of a different number of unit cells (Unit cell-1 in Figure 10(A)) under simple shear

| RVE   | Homogenized first PK stress $\bar{P}$ | Homogenized tangent moduli $\bar{\lambda}$ | Homogenized stored energy $\bar{\psi}$ |
|-------|--------------------------------------|----------------------------------------|--------------------------------------|
| 1×1   | 0.0128                               | [26.1954, -0.6689, 0.3549, 8.3450]      | 2.423 × 10^{-3}                      |
| 1×2   | 0.1893                               | [0.3549, 0.0503, 0.2038, 0.9365]        |                                      |
| 2×1   | 0.1953                               | [8.3450, -0.9698, 0.9365, 21.0161]      |                                      |
| 2×2   | 0.0598                               |                                        |                                      |

Abbreviation: RVE, representative volume element.

The same shear band can be observed. Table 7 lists the homogenized quantities such as homogenized stress, tangent moduli, and stored elastic energy. Again, it can be seen that all the homogenized quantities match fairly well with each other.

4 | MULTISCALE STABILITY

A basic assumption in the homogenization analysis is that one unit cell can serve as the fundamental periodic cell during the entire loading process and can be taken as RVE. For finitely strained nonlinear periodic materials, this assumption, however, may be violated. Upon loading, for instance, buckling with wavelength possibly across arbitrary length can happen at the microscale, which will lead to the violation of the assumption that one unit cell can serve as the fundamental cell. If the buckling mode is periodic, a fundamental cell can still be found that may consist of more than one unit cell, while when the buckling mode is aperiodic, there is no fundamental periodic cell that can be further used. From a macroscopic viewpoint, though polyconvexity in the sense of Ball of the underlying material phases can be guaranteed
FIGURE 11  Deformed shapes and equivalent plastic strain ($\alpha$) distributions of the RVE consisting of different number of unit cells (unit cell-1) under simple shear. RVE, representative volume element

FIGURE 12  Deformed shapes and equivalent plastic strain ($\alpha$) distributions of the RVE with different unit cells under simple shear. RVE, representative volume element

by using appropriate constitutive models, which ensures the rank-1 convexity, the homogenized macroscopic material may still lose rank-1 convexity.\textsuperscript{34} As shown in the previous studies, there exists a close connection between microscale buckling and macroscale loss of rank-1 convexity, that is, long wavelength buckling on the microscale corresponds to the loss of rank-1 convexity of the homogenized incremental moduli at macroscale.\textsuperscript{37,40} It is also noted that the microinstability (short wavelength buckling) occurs either before or simultaneously with the macroinstability (long wavelength buckling).\textsuperscript{37,40} Compared with the macrostability check, where a rank-1 convexity examination of the homogenized incremental moduli is only needed, the microstability check is much more computationally demanding, since the length
FIGURE 13 Macroscopic deformation gradient—stress curves of the RVE analysis with different unit cells under simple shear. RVE, representative volume element

TABLE 6 Homogenized quantities from the elastoplastic RVE of different unit cells under simple shear

| RVE        | Homogenized first PK stress \([\bar{P}]\) | Homogenized tangent moduli \([\bar{A}]\) | Homogenized stored energy \(\bar{\psi}^e\) |
|------------|----------------------------------------|----------------------------------------|----------------------------------------|
| Unit cell-1| 0.0128 \[0.1893, 0.1953, 0.0598\]       | \[26.1954, -0.6689, 0.3549, 8.3450\]  | \[2.423 \times 10^{-3}\]             |
| Unit cell-2| 0.0129 \[0.1893, 0.1953, 0.0600\]       | \[26.1923, -0.6768, 0.3458, 8.3341\]  | \[2.448 \times 10^{-3}\]             |

Abbreviation: RVE, representative volume element.

scale of buckling mode is not a priori known. Note that the surface buckling type instability at the matrix-inclusion/void boundary, which is of short wavelength, is not included in the microscale stability examination and interested readers are referred to Reference 57.

4.1 Microscale stability

For rate-independent solids, the stability is governed by Hill’s stability criterion.58 The principal solution branch ceases to be stable when the functional \(\beta(\lambda)\) defined by

\[
\beta(\lambda) = \min_{\bar{v}} Q(\bar{v}; \Omega) \quad \text{with} \quad Q(\bar{v}; \Omega) = \frac{\int_{\Omega} \nabla \bar{X} \bar{v} : \bar{A} : \nabla \bar{X} \bar{v} \, dV}{\int_{\Omega} \nabla \bar{X} \bar{V} : \nabla \bar{X} \bar{V} \, dV}
\]

(44)

loses positive definiteness, where \(\bar{v}\) is taken from the kinematically admissible displacement variation space \(H^1_0(\Omega)\) for the corresponding macroscale boundary value problem. For periodic solids of infinite extent \((\Omega \to \mathbb{R}^d)\), \(\bar{v}\) is taken from locally integrable, bounded functions that ensure the finiteness of the ratio \(Q\), and correspondingly the minimum in Equation (44) is taken as infimum. In Equation (44), \(\bar{V}\) denotes the complex conjugate of \(\bar{v}\) and \(\lambda\) stands for the loading parameter. The tensor \(\bar{A}\) represents the tangent moduli (Equation (25)) under the loading parameter \(\lambda\) with the same periodicity as one unit cell. It was shown in Reference 37 that this infimum \(\beta(\lambda)\) can be computed through Bloch wave analysis, where the calculation is carried out within the RVE (e.g., one unit cell) \(\Omega_0^u\) and is expressed as
Illustration of three different ways of choosing RVE from the porous periodic elastoplastic material. RVE, representative volume element

(A) (B) (C)

FE meshes of three RVEs of the porous elastoplastic periodic material. RVE, representative volume element

RVE-1 ($n_{ele} = 3150$) RVE-2 ($n_{ele} = 13200$) RVE-3 ($n_{ele} = 7584$)

where $v_B$ is the Bloch wave representing the eigenmode in which $i = \sqrt{-1}$, $u$ is a periodic function with the same periodicity as the RVE, that is, $u(X + c_i a_i) = u(X)$ with $c_i$ arbitrary integers and $a_i$ the $i$th periodic lattice vector ($i = 1, \ldots, d$), while the wavevector $k$ is chosen in the reciprocal space spanned by the reciprocal bases $b_i$ ($i = 1, \ldots, d$) defined by $a_i \cdot b_j = 2\pi \delta_{ij}$, that is, $k = \sum_{i=1}^{d} k_i b_i$. For example, Figure 17(A, B) illustrate two different lattice spaces and their corresponding reciprocal lattice spaces.

It is worth noting that two physically different types of buckling modes exist in the neighborhood of $k = 0$, that is, the long wavelength instability with $k \rightarrow 0$ that leads to the loss of rank-1 convexity of the homogenized tangent moduli at the macroscale (see Section 4.2), and a short wavelength buckling mode with $k = 0$ which has the same periodicity as the RVE. For short wavelength buckling, the infimum in Equation (45) is achieved at $k = 0$ and the microscale stability surface, plotted as $\beta(\lambda)$ against $k_1$ and $k_2$ (for 2D case), is continuous at origin ($k = 0$) at critical loading parameter $\lambda_c$. However, for long wavelength buckling, the infimum in Equation (45) is not reachable and can only be computed as the limit $k \rightarrow 0$, and the microscale stability surface is discontinuous at origin (singular point). This is the reason for using infimum instead of minimum in Equation (45). Interested readers are referred to References 37, 40 for further theoretical details.
FIGURE 16 Deformed shapes and equivalent plastic strain (\(\alpha\)) distributions of different RVEs under simple shear. RVE, representative volume element.

TABLE 7 Homogenized quantities from the different porous elastoplastic RVEs under simple shear

| RVE   | Homogenized first PK stress \([\bar{P}]\) | Homogenized tangent moduli \([\bar{A}]\) | Homogenized stored energy \(\bar{\psi}\) |
|-------|------------------------------------------|------------------------------------------|---------------------------------|
| RVE-1 | 0.0393                                   | 9.5021, -0.1584, 0.0571, 1.4065           | 1.389 \times 10^{-3}           |
|       | 0.0748                                   | -0.1584, 0.0372, -0.0200, -0.1788         |                                |
|       | 0.0817                                   | 0.0571, -0.0200, 0.0607, 0.1146            |                                |
|       | 0.0692                                   | 1.4065, -0.1788, 0.1146, 3.7513            |                                |
| RVE-2 | 0.0393                                   | 9.5020, -0.1586, 0.0572, 1.4064            | 1.388 \times 10^{-3}           |
|       | 0.0748                                   | -0.1582, 0.0370, -0.0201, -0.1783          |                                |
|       | 0.0817                                   | 0.0572, -0.0201, 0.0606, 0.1150            |                                |
|       | 0.0692                                   | 1.4064, -0.1783, 0.1150, 3.7504            |                                |
| RVE-3 | 0.0393                                   | 9.5020, -0.1586, 0.0569, 1.4064            | 1.389 \times 10^{-3}           |
|       | 0.0748                                   | -0.1586, 0.0373, -0.0200, -0.1796          |                                |
|       | 0.0817                                   | 0.0569, -0.0200, 0.0607, 0.1138            |                                |
|       | 0.0692                                   | 1.4064, -0.1796, 0.1138, 3.7513            |                                |

Abbreviation: RVE, representative volume element.

4.1.1 Wavevector (\(k\)) space

For Bloch wave analysis, the sufficient wavevector space to be examined can be chosen as the primitive cell (smallest periodic cell or unit cell) in the reciprocal space, and the Bloch wave functions with wavevectors outside the primitive cell are all represented due to the periodicity. To see this, consider a 2D unit cell with periodic vectors \(a_1\) and \(a_2\). In the reciprocal lattice space, which is periodic with respect to periodic bases \(b_1\) and \(b_2\) (note that \(a_i \cdot b_j = 2\pi \delta_{ij}\)), by definition, for any wavevector \(k\), there is a translational vector \(T = i_1 b_1 + i_2 b_2\) (\(i_1, i_2 \in \mathbb{Z}\) = set of integer) such that \(k = k_{PC} + T\) with \(k_{PC}\) a wavevector in the primitive cell, see Figure 18(A). As a result, the Bloch wave function with wavevector \(k\) is expressed as

\[v_B = e^{ik \cdot x} u_k.\] (46)
where a subscript \( k \) is used for the periodic function \( u_k(X) = u(X) \) to make it clear that this periodic function is based on the wavevector \( k \). Note that the function \( u_k(X) \) is periodic in the lattice space, that is, \( u_k(X + q_1a_1 + q_2a_2) = u_k(X) \) for any \( q_1, q_2 \in \mathbb{Z} \). Thus, it can be shown that

\[
v_B = e^{ik \cdot X} u_k = e^{ik_{pc} \cdot X} e^{T \cdot X} u_k = e^{ik_{pc} \cdot X} u_{k_{pc}},
\]  

(47)

where

\[
u_{k_{pc}}(X) = e^{T \cdot X} u_k(X)
\]  

(48)

is another periodic function in the lattice space, since \( \forall q'_1, q'_2 \in \mathbb{Z} \)

\[
u_{k_{pc}}(X + q'_1a_1 + q'_2a_2) = e^{T(X + q'_1a_1 + q'_2a_2)} u_k(X + q'_1a_1 + q'_2a_2) = e^{T \cdot X} u_k(X) = u_{k_{pc}}(X).
\]  

(49)

Thus, Equations (47) and (49) show that for any wave vector \( k \) in the reciprocal space, the Bloch wave function \( v_B \) can be equivalently expressed in terms of wavevector \( k_{pc} \) in the primitive cell and a corresponding periodic function that is still periodic w.r.t unit cell in the lattice space. From this discussion, it is clear that for a Bloch wave function representation, the wavevector \( k \) space can simply and sufficiently be chosen as any primitive cell in the reciprocal space. Thus, for any parallelogram-shaped RVE, the wavevector \( k \) space can always be chosen as \( k_1, k_2 \in [0, 1) \). It is noted that as a special case, the first Brillouin zone, which is mostly used in solid-state physics,\(^5^9\) is also a primitive cell (see Figure 18(B)) in the reciprocal space, and thus can also be used as the wavevector space for evaluating \( \beta(\lambda) \) in Equation (45). In this study, the primitive cell with \( k_1, k_2 \in [0, 1) \) is used, as shown in Figure 18(A).
4.1.2 Interpretation of the Bloch wave function as buckling mode

The equivalence between Equations (44) and (45) has been established in Reference 37. However, since the buckling mode in Equation (44) is in real physical space, it is not clear how the complex-valued Bloch wave function can be treated as the buckling mode or how a real-valued mode can be extracted from the Bloch wave function $v_B$. As shown in Reference 37 that if $X$ is a subsequence in $H^1_0(\Omega)$ and $X \oplus iX$ is its complexification, then

$$\min_{v \in X \oplus iX} Q(v; \Omega) = \min_{v \in X} Q(v; \Omega).$$

(50)

For further exposition, the proof of this assertion is detailed below.

**Proof.** First, it is clear that $\min_{v \in X \oplus iX} Q(v; \Omega) \leq \min_{v \in X} Q(v; \Omega)$ since $X$ is a subset of $X \oplus iX$. Thus, it is enough to show that $\min_{v \in X} Q(v; \Omega) \leq \min_{v \in X \oplus iX} Q(v; \Omega)$. To this end, for any $v \in X \oplus iX$, write

$$v = \text{Re}(v) + i \text{Im}(v) = w_1 + iw_2.$$  

(51)

Substituting Equation (51) into $Q(v; \Omega)$ defined in Equation (44), using the major symmetry of $A$, gives

$$Q(v; \Omega) = \frac{\int_{\Omega} \nabla w_1 : A : \nabla w_1 \, dV + \int_{\Omega} \nabla w_2 : A : \nabla w_2 \, dV}{\int_{\Omega} \nabla w_1 : \nabla w_1 \, dV + \int_{\Omega} \nabla w_2 : \nabla w_2 \, dV}.$$  

(52)

Since $w_1, w_2 \in X$, assuming that $\beta = \min_{v \in X} Q(v; \Omega)$ and $\beta_1 \overset{\text{def}}{=} Q(w_1; \Omega)$ and $\beta_2 \overset{\text{def}}{=} Q(w_2; \Omega)$ gives $\beta_1 \geq \beta$ and $\beta_2 \geq \beta$. Without loss of generality, assume that $\beta_1 \leq \beta_2$. Thus,

$$\beta \leq \beta_1 \leq \frac{\int_{\Omega} \nabla w_1 : A : \nabla w_1 \, dV + \int_{\Omega} \nabla w_2 : A : \nabla w_2 \, dV}{\int_{\Omega} \nabla w_1 : \nabla w_1 \, dV + \int_{\Omega} \nabla w_2 : \nabla w_2 \, dV} \leq \beta_2,$$

(53)

which results in $\min_{v \in X} Q(v; \Omega) \leq \min_{v \in X \oplus iX} Q(v; \Omega)$ with the equality holding only when $\beta_1 = \beta_2 = \beta$. That means, if the minimum $\min_{v \in X} Q(v; \Omega)$ is reached by a set of vectors $Z \subseteq X$, the minimum $\min_{v \in X \oplus iX} Q(v; \Omega)$ is reached by the complexification of the same particular set, that is, $v \in Z \oplus iZ$. 

The above proof demonstrates that if the minimum of $Q(v; \Omega)$ is reached in the complex domain, both the real part and the imaginary part belong to the same set which leads to the minimum value of $Q(v; \Omega)$ in the real domain. In terms of the Bloch wave analysis, this means that if zero value of the function $\inf_k \min_u Q(v_B(k, u); \Omega^\mu)$ is detected by a complex-valued
Bloch wave function $v_B$, then the buckling mode can be either obtained from the real part or the imaginary part, since both are from the same set and differ only by a phase shift.

### 4.1.3 Remarks

As mentioned above, the buckling modes can be of any finite wavelength or even aperiodic. This poses a significant challenge in the stability analysis of periodic materials since the solution belongs to the entire (infinite) lattice space, and FE model including multiple unit cells, has to be employed if stability is directly investigated, as proposed in Reference 46. However, expressing the buckling modes in terms of the Bloch wave functions simplifies the solution process, since instead of searching the entire lattice space, the Bloch wave solutions are sought using FE model with only one unit cell. However, in this case, all $k$ values belonging to the primitive cell in the reciprocal space that theoretically consists of infinite points have to be examined. From a finite element analysis viewpoint, the Bloch function method makes the problem computationally tractable, as it makes it possible to determine the stability of periodic materials while employing only one unit cell as RVE, which would otherwise become computationally intractable if the direct method presented in Reference 46 is employed. Furthermore, if the microscale stability is examined by structural stability analysis with an increasing number of unit cells in RVE as proposed in Reference 46, this strategy will still fail to capture aperiodic buckling modes. Thus, this direct stability examination is both computationally expensive and inaccurate. Indeed, as shown in Reference 37, it is only when the search space includes RVE that consists of an infinite number of unit cells will the direct method in Reference 46 give the same result as the Bloch wave analysis on a unit cell.

### 4.2 Macroscale stability

As a measure of the macroscopic stability, the rank-1 convexity of the homogenized tangent moduli ensures the absence of discontinuities in the deformation gradient field on the macroscale. Macroscopic stability can be assessed by examining the positive definiteness of the ellipticity indicator $B(\lambda)$ defined by

$$B(\lambda) = \min_{\bar{m}, \bar{M}} \langle \bar{m} \otimes \bar{M} : \bar{\lambda} : (\bar{m} \otimes \bar{M}) \rangle,$$

where $\bar{m}$ and $\bar{M}$ span over all possible directions with $||\bar{m}|| = ||\bar{M}|| = 1$. A recent study has also shown that upon the loss of rank-one convexity there is not always a discontinuous/localized deformation pattern on the bifurcated branch. The presence or absence of localized deformation depends on the stability of the bifurcated branch. When there is a discontinuous deformation corresponds to the loss of rank-1 convexity, that is, $B(\lambda) = 0$, the corresponding minimizing vector $\bar{M}$ represents the normal to the curves across which the jump discontinuities appear and $\bar{m}$ determines the nature of the discontinuous mode (simple shear if $\bar{m}$ is orthogonal to $\bar{M}$ or pure splitting if $\bar{m}$ is parallel to $\bar{M}$ or mixture otherwise).

As has been proved in Reference 37, the following inequality holds

$$\beta(\lambda) \leq \beta(\lambda; k \to 0) \leq B(\lambda).$$

Equation (55) implies that if the microscopic stability is preserved, that is, $\beta(\lambda) > 0$, the homogenized macroscopic material is rank-1 convex. It is noted that the first inequality in Equation (55) is straightforward since the $k$ space in $\beta(\lambda)$ includes the case $k \to 0$. Besides, it is also shown in Reference 37 that the loss of rank-1 convexity corresponds to a long wavelength microscale buckling, that is,

$$B(\lambda) = 0 \text{ if } \beta(\lambda; k \to 0) = 0.$$

As a result, the detection of long wavelength buckling can be more efficiently carried out by rank-1 convexity examination compared with the Bloch wave analysis.

### 4.3 Implementation details—Bloch analysis

In this section, three numerical methods are presented that can be used for microscale stability analysis described in Section 4.1 using Bloch waves. Since only zero values of the stability indicator $\beta(\lambda)$ are of interest, the normalization
by the denominator in Equation (44) can be ignored. To this end, the discrete form of Equation (45) can be expressed as

\[ \beta(\lambda) = \inf_k \min_u F(v_B) \]  

(57)

with

\[ F(v) = v^T K_T v \quad \text{and} \quad v_B(k, u) = e^{i k \cdot u}, \]  

(58)

where the symbol * denotes the complex conjugate transpose. All the presented methods aim at finding the lowest value of loading parameter \( \lambda = \lambda_c \), also known as critical load/point, at which the quadratic stability functional in Equation (57) loses its positive definiteness. The first two methods are based on condensation schemes and the last method is based on the null-space projection scheme. Note that this is a case of a constrained eigenvalue problem, where constraints are determined by the Bloch conditions.

### 4.3.1 Condensation method—I

In this method, the DOFs (microscale displacement field) of the underlying RVE are partitioned into three groups, \( v_a \) on the negative side, \( v_b \) on the positive side and \( v_i \) of the interior nodes, that is,

\[ v = \begin{bmatrix} v_a \\ v_b \\ v_i \end{bmatrix} \]  

(59)

and the tangent stiffness matrix \( K_T \) (Equation (25)) at the loading step (\( \lambda \)) of interest is accordingly partitioned as

\[ K_T = \begin{bmatrix} K_{aa} & K_{ab} & K_{ai} \\ K_{ba} & K_{bb} & K_{bi} \\ K_{ia} & K_{ib} & K_{ii} \end{bmatrix}. \]  

(60)

Since the buckling mode can be represented by the Bloch wave function, that is, Equation (45), it can be shown that the DOFs on the positive side are related to the DOFs on the negative side by

\[ v_b = M(k)v_a. \]  

(61)

where, for instance, in the case of parallelogram RVE (see Figures 2(A) or 3(A)) the matrix \( M = M(k) \) contains nonzero elements of the form \( e^{i k \cdot a_1}, e^{i k \cdot a_2}, \) and \( e^{i k \cdot (a_1 + a_2)} \) where \( a_1 \) and \( a_2 \) are two periodic vectors, that is,

\[ M(k) = \begin{bmatrix} e^{i k \cdot a_1} & \cdots & e^{i k \cdot a_2} \\ \vdots & \ddots & \vdots \\ e^{i k \cdot (a_1 + a_2)} & \cdots & e^{i k \cdot (a_1 + a_2)} \end{bmatrix}. \]  

(62)
where the first matrix block represents the Bloch periodic boundary condition on the left and right pairing sides and the second matrix block represents the bottom and top pairing sides, while the third block represents the boundary conditions on the corner nodes, see Equation (45) and Figure 3(A), where corner node 1 is taken as on the negative side while corner nodes 2, 3, 4 are taken as on the positive side and are related to the corner node 1 by the Bloch periodic conditions. The Bloch wave analysis for microscale stability then seeks the first point during the loading process where the eigenvalue(s) $\beta$ of the tangent stiffness matrix $K_T$ with eigenmode satisfying Equation (45) is (are) zero, that is,

\[ \text{Find the lowest value of the loading parameter } \lambda_c \text{ such that the minimum of the eigenvalues } \beta(\lambda_c) = 0 \text{ with } \beta \text{ defined as} \]

\[
\begin{bmatrix}
K_{aa} & K_{ab} & K_{ai} \\
K_{ba} & K_{bb} & K_{bi} \\
K_{ia} & K_{ib} & K_{ii}
\end{bmatrix}
\begin{bmatrix}
v_a \\
v_b \\
v_i
\end{bmatrix}
= \beta
\begin{bmatrix}
v_a \\
v_b \\
v_i
\end{bmatrix}
\text{ with } v_b = M v_a
\]

(63)

which leads to

\[
\begin{bmatrix}
K_{aa} & K_{ab} & K_{ai} \\
K_{ba} & K_{bb} & K_{bi} \\
K_{ia} & K_{ib} & K_{ii}
\end{bmatrix}
\begin{bmatrix}
v_a \\
v_b \\
v_i
\end{bmatrix}
H
= \beta H
\begin{bmatrix}
v_a \\
v_b \\
v_i
\end{bmatrix}
\text{ with } H = \begin{bmatrix} I & 0 \\ M & 0 \\ 0 & I \end{bmatrix}.
\]

(64)

where $I$ is an identity matrix of appropriate size. Due to the linear independency of the columns in matrix $H$, the system of equations in Equation (64) is equivalent to

\[
\begin{bmatrix}
\hat{K}_{aa} & \hat{K}_{ai} \\
\hat{K}_{ia} & \hat{K}_{ii}
\end{bmatrix}
\begin{bmatrix}
v_a \\
v_i
\end{bmatrix}
= \beta G
\begin{bmatrix}
v_a \\
v_i
\end{bmatrix}
\text{ with } G = H^T H,
\]

(65)

where

\[
\begin{align*}
\hat{K}_{aa} &= K_{aa} + K_{ab} M + M^T K_{ba} + M^T K_{bb} M \\
\hat{K}_{ai} &= K_{ai} + M^T K_{bi} \\
\hat{K}_{ia} &= K_{ia} + K_{ib} M \\
\hat{K}_{ii} &= K_{ii}
\end{align*}
\]

(66)

and $^*$ is the complex conjugate transpose since $M$ is a complex-valued matrix. It should be noted that since the non-zero entries of the matrix $M$ are $e^{ikL}$ with $L$ some periodic translation vectors (e.g., $a_1, a_2$ for the nodes on the side while $a_1 + a_2$ for some corner nodes), the matrix $M^T M$ is a diagonal matrix with most of the entries equal to 1 and a few entries corresponding to slave corner node DOFs to be two or three depending on different RVE shapes (see Figure 3 and remarks in Section 2.1.1). Hence, the matrix $G$ is a diagonal matrix, as well. As a result, the original eigenvalue problem, Equation (63), is equivalently transformed to the following condensed eigenvalue problem

\[
G^{-1}
\begin{bmatrix}
\hat{K}_{aa} & \hat{K}_{ai} \\
\hat{K}_{ia} & \hat{K}_{ii}
\end{bmatrix}
\begin{bmatrix}
v_a \\
v_i
\end{bmatrix}
= \beta
\begin{bmatrix}
v_a \\
v_i
\end{bmatrix},
\]

(67)

where the invertibility of the matrix $G$ is obvious.

Remark. : Since the first bifurcation point is of interest, that is, the loading parameter $\lambda$ at which the minimum eigenvalue $\beta = 0$, the existence of zero (or negative) eigenvalue of the matrix

\[
G^{-1}
\begin{bmatrix}
\hat{K}_{aa} & \hat{K}_{ai} \\
\hat{K}_{ia} & \hat{K}_{ii}
\end{bmatrix}
\]

(68)
is equivalent to the existence of zero (or negative) eigenvalue of the matrix

\[
\begin{bmatrix}
\hat{K}_{aa} & \hat{K}_{ai} \\
\hat{K}_{ia} & \hat{K}_{ii}
\end{bmatrix}
\]  

(69)

due to the positive definiteness of the matrix \( G \) or equivalently \( G^{-1} \). Moreover, even though in general the eigenvectors of the matrix in Equation (68) are different from those of the matrix in Equation (69), the eigenvectors corresponding to the buckling mode, that is, the eigenvector corresponding to zero eigenvalues, are the same for the systems in Equations (68) and (69). As a result, eigen analysis can be carried out for the matrix in Equation (69).

4.3.2 Condensation method—II

The condensation method in Section 4.3.1 implements the Bloch wave analysis by condensing out \( v_b \), that is, the degrees of freedom corresponding to the positive side. To further reduce the computational cost, Triantafyllidis et al.\(^40\) proposed another condensation method, where the eigen analysis is carried out for a matrix of the same size as \( K_{aa} \). From Equation (63), assuming that the analysis is carried out at the zero eigenvalue, that is, at \( \beta = 0 \), results in

\[
K_{ia}v_a + K_{ib}v_b + K_{ii}v_i = 0.
\]  

(70)

From Equation (70), one part of the eigenvector \( (v_i) \) can be expressed in terms of \( v_a \) as

\[
v_i = Wv_a \text{ with } W = -K_{ii}^{-1}(K_{ia} + K_{ib}M),
\]  

(71)

where the relation \( v_b = Mv_a \) is used. Thus, to use this condensation method the inverse \( K_{ii}^{-1} \) have to be calculated. Note that this may lead to increase memory requirements during the solution process, as the inverse of sparse matrices is, in general, not sparse. With eigenvector components \( v_b \) and \( v_i \) expressed in terms of \( v_a \), the original eigenvalue equation in Equation (63) can be rewritten as

\[
\begin{bmatrix}
K_{aa} & K_{ab} & K_{ai} \\
K_{ba} & K_{bb} & K_{bi} \\
K_{ia} & K_{ib} & K_{ii}
\end{bmatrix}
\begin{bmatrix}
\hat{H}v_a \\
\hat{H}v_b \\
\hat{H}v_i
\end{bmatrix} = \beta \begin{bmatrix} I \\ M \\ W \end{bmatrix},
\]  

(72)

which, due to the linear independency of the column vectors in matrix \( \hat{H} \), is equivalent to

\[
\hat{K}v_a = \beta Dv_a \text{ with } D = \hat{H}^\dagger \hat{H}
\]  

(73)

or

\[
D^{-1}\hat{K}v_a = \beta v_a,
\]  

(74)

where

\[
\hat{K} = \hat{H}^\dagger K_{aa}\hat{H} = K_{aa} + K_{ab}M + K_{ai}W + M^\dagger (K_{ba} + K_{ib}M + K_{bi}W)
\]  

\[
= K_{aa} + K_{ab}M + M^\dagger K_{ba} + M^\dagger K_{bb}M - (K_{ii} + M^\dagger K_{bi})K_{ii}^{-1}(K_{aa} + K_{ib}M).
\]  

(75)

As can be seen, the size of the matrix in the eigen analysis is significantly reduced by using the conditions in Equation (70). In addition, the inversion of \( K_{ii} \) is only needed once at each loading step. Thus, this method can be more efficient than the one in Section 4.3.1, especially when the sampling grid in the \( k \)-space is large. Moreover, when the first bifurcation point is of interest, the eigen analysis of matrix \( \hat{K} \) can be carried out to search for a zero (or negative) eigenvalue instead of the original matrix \( D^{-1}\hat{K} \) due to the positive definiteness of matrix \( D \) or \( D^{-1} \). The positive definiteness of
\( \mathbf{D} \) can be established, as for any vector \( \mathbf{v}_a \neq 0 \)

\[
\mathbf{v}_a^T \mathbf{D} \mathbf{v}_a = \mathbf{v}_a^T (\mathbf{I} + \mathbf{M}^T \mathbf{M} + \mathbf{W}^* \mathbf{W}) \mathbf{v}_a = ||\mathbf{v}_a||^2 + ||\mathbf{v}_b||^2 + ||\mathbf{v}_i||^2 > 0.
\] (76)

Similarly, the buckling mode, that is, the eigenvector corresponding to zero eigenvalue, can also be obtained by eigen analysis on matrix \( \hat{\mathbf{K}} \) instead of \( \mathbf{D}^{-1} \hat{\mathbf{K}} \).

4.3.3  ||  Null-space projection method

In this method, the constraints on the eigenmode, that is, Equation (45)\textsuperscript{2}, are expressed as

\[ \mathbf{C} \mathbf{v} = \mathbf{0} \] (77)

where matrix \( \mathbf{C} \) is of size \( N_c \times N \) such that \( \text{rank}(\mathbf{C}) = N_c \), with \( N_c < N \) the number of constraints, and \( N \) the total number of DOFs. From Equation (77), it is clear that the eigenvectors should belong to the null space \( \mathcal{N}(\mathbf{C}) \) of the constraint matrix \( \mathbf{C} \) with \( \dim(\mathcal{N}(\mathbf{C})) = N - N_c \). As a result, the eigenvector/buckling mode \( \mathbf{v} \) should be spanned in a space consisting of \( (N - N_c) \) bases vectors \( \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_{N-N_c} \) of \( \mathcal{N}(\mathbf{C}) \), that is,

\[ \mathbf{v} = \mathbf{Y} \mathbf{z} \] (78)

where \( \mathbf{z} \in \mathbb{R}^{N-N_c} \). Hence, with the null-space based representation of the eigenvector \( \mathbf{v} \), the constrained eigen analysis (Equation (63)) becomes

\[ \mathbf{K}_T \mathbf{Y} \mathbf{z} = \beta \mathbf{Y} \mathbf{z}. \] (79)

To further proceed, the basis matrix \( \mathbf{Y} \) of \( \mathcal{N}(\mathbf{C}) \) is needed. To this end, the QR decomposition of \( \mathbf{C}^* \) matrix is carried out, which gives

\[ \mathbf{C}^* = \mathbf{QR} \text{ with } \mathbf{Q} = \begin{bmatrix} \mathbf{Q}_1_{N \times N_c} & \mathbf{Q}_2_{N \times (N-N_c)} \end{bmatrix} \text{ and } \mathbf{R} = \begin{bmatrix} \mathbf{R}_1_{N_c \times N_c} \\ \mathbf{0}_{(N-N_c) \times N_c} \end{bmatrix} \] (80)

with an illustration shown in Figure 19. From Figure 19 and by the definition of QR decomposition, it is known that the columns in \( \mathbf{Q} \) matrix are orthonormal vectors and columns in \( \mathbf{Q}_1 \) form the basis for \( \mathcal{R}(\mathbf{C}^*) \), that is, the range space of \( \mathbf{C}^* \), while the columns in \( \mathbf{Q}_2 \) form the basis for \( \mathcal{N}(\mathbf{C}) \), that is, the null space of \( \mathbf{C} \). Therefore, \( \mathbf{Y} \) can be chosen as \( \mathbf{Q}_2 \) and as a result, Equation (79) can be equivalently expressed as

\[ \mathbf{Q}_2^T \mathbf{K} \mathbf{Q}_2 \mathbf{z} = \beta \mathbf{z}. \] (81)

where the orthonormality of the column vectors in \( \mathbf{Q}_2 \) is used. This projected eigenvalue problem is then solved and the eigenvector \( \mathbf{v} \) (buckling mode) can be simply recovered by \( \mathbf{v} = \mathbf{Q}_2 \mathbf{z} \).

4.3.4  ||  Remarks

With the Bloch type boundary conditions rephrased in a constraints matrix in the null-space projection method, it has been shown that this method is particularly useful for the case where the boundary nodal degree of freedoms are not properly aligned, for example, in isogeometric analysis.\textsuperscript{50} In all the three methods, for buckling modes that are larger than one unit cell, that is, \( \mathbf{k} \neq \mathbf{0} \), the rigid-body motion is implicitly suppressed by the Bloch boundary conditions (Equation (45)\textsuperscript{2}), so there is no need for adding extra constraints. However, for buckling mode that is periodic with respect
to one unit cell, that is, $k = 0$, extra constraints are needed for constraining the rigid-body translation, for example, fixing one arbitrary point. For instance, when $k \neq 0$, $N_c = 2m$ for 2D case in Equation (78) where $m$ denotes the number of pairs of nodes lying on the negative and positive boundary sides (see Equation (15)), while when $k = 0$, $N_c = 2m + 2$ where an arbitrary node in the domain is fixed.

5 | NUMERICAL EXAMPLES—MULTISCALE STABILITY

The purpose of this section is to demonstrate the efficacy of the proposed framework for the multiscale stability analysis using representative test cases. In the first example, the three methods presented in Section 4.3 are used and compared in detecting the multiscale instability point, while in the rest of the following examples, the null-space projection method is used for the Bloch wave analysis. Both strain driven and stress driven homogenization frameworks are employed for studying the multiscale stabilities of different microstructures. The goal of multiscale stability analysis is to determine the first bifurcation point and the buckling mode at the first bifurcation point. For the Bloch wave analyses, the $k$-space mesh with $(k_1, k_2) \in [0,1] \times [0,1]$ consists of a $100 \times 100$ uniform mesh over $[0,1] \times [0,1]$ and $100 \times 100$ uniform meshes in the three refined zones $(0,0.01) \times (0.01,1]$, $(0.01,1] \times (0,0.01)$, and $(0,0.01) \times (0,0.01)$. For the rank-1 convexity check, the positive definiteness of the indicator $B(\lambda)$ in Equation (54) is examined at each loading step at every $\pi/720$ radian increment in both $\mathbf{m}$ and $\mathbf{M}$ space. After the critical load is approximately located, bisection analyses are further carried out to further refine the accuracy of the detected first bifurcation point $(\lambda_c)$ based on the selected $k$-mesh.

5.1 | Example-1: Comparison of the three methods

The first example compares the three methods presented in Section 4.3. Specifically, a square unit cell of unit size with a central circular hole of radius $r = 0.4$ is considered with matrix material following neo-Hookean model in Equation (43) with $\kappa = 166.67$ and $\mu = 35.71$. Uniaxial load is considered where $\theta = 0^\circ$ and $\phi = \pi/2$ in Equations (32) and (35), respectively, under stress driven framework. For the verification of the stress driven loop, Figure 20 plots the homogenized Kirchhoff stress in the principal direction, that is, $\mathbf{\tau}' = \mathbf{\tau}$ in Equation (32), where it can be seen that both $\tau_{12} = \tau_{21} = 0$ and $\tau_{11} = 0$ in the loading process. The microscale stability surfaces in Figures 21 and 22 are plotted where the stability indicator $\gamma_k$ is defined as the minimum eigenvalues ($\beta$) in Equation (63) with wavevector ($k$) at the first bifurcation load from different methods. As discussed in Sections 4.3.1 and 4.3.2, the multiscale stability analysis (seeking first bifurcation load and buckling mode) is not affected by either including $G^{-1}$ (or $D^{-1}$) in Equation (67) (or Equation 74) or excluding these matrices in eigen analysis. Excluding $G^{-1}$ and $D^{-1}$ in the two condensation methods, the first bifurcation loads detected using all the three methods are the same (with loading step size $\Delta \lambda = 7.5 \times 10^{-5}$) and the three buckling modes that are also the same, see Figure 21. However, the microscale stability surfaces can be different, as expected, see Figure 21(A,B). To demonstrate the equivalency of the three methods, the matrices $G^{-1}$ and $D^{-1}$ are included in the two condensation methods and the Bloch wave analyses are carried out again with the results shown in Figure 22. This result shows that not only the same first bifurcation load and buckling mode are obtained from the three methods, the microscale stability surfaces are also identical. It is also noted that a clear discontinuity at the origin $(k_1, k_2) = (0, 0)$.
FIGURE 20  Homogenized Kirchhoff stresses in the principal direction at load steps

Condensation method – I: $\lambda_c = 2.4620$

Condensation method – II: $\lambda_c = 2.4620$

Null-space projection method: $\lambda_c = 2.4620$

FIGURE 21  Microscale stability surfaces and buckling modes at first bifurcation points ($\lambda_c$) using different methods with $G^{-1}$ and $D^{-1}$ excluded in Equations (67) and (74) (left column: microscale surface, right column: buckling mode)
FIGURE 22  Microscale stability surfaces and buckling modes at first bifurcation points ($\lambda_c$) using different methods with $G^{-1}$ and $D^{-1}$ included in Equations (67) and (74) (left column: microscale surface, right column: buckling mode)

FIGURE 23  Illustration of different choices of RVE for composite with inclined circular holes. RVE, representative volume element
can be observed in the microscale stability surfaces in Figure 22. This discontinuity implies that the buckling mode with periodicity of one unit cell is not present at the first bifurcation load.

### 5.2 Example-2: Equivalency of different RVEs in multiscale stability analysis

The second example considers periodic material with inclined circular holes of radius $r = 0.4$, see Figure 23, where the overall porous material can be represented by different periodic cells. The matrix material again follows neo-Hookean model (Equation (43)) with $\kappa = 166.67$ and $\mu = 35.71$. A constrained compression along an inclined angle ($30^\circ$) is considered under strain driven framework. The macroscopic deformation gradient $\bar{F}$ is applied as

$$\bar{F} = Q \begin{bmatrix} 1 & 0 \\ 0 & \lambda \end{bmatrix} Q^T,$$

where the bases transformation matrix $Q$ is given in Equation (32) with $\theta = 30^\circ$ and $\lambda$ represents loading parameter that decreases from 1 indicating compression.

Among the three RVEs (parallelogram, hexagon, and rectangle), the parallelogram and hexagon are both the (smallest) fundamental unit cells of the same size, while the rectangle-shaped RVE is twice the size as compared with other RVEs. For parallelogram and hexagon-shaped RVEs, the periodic vectors $a_1$ and $a_2$ are both unit vectors with the angle between them equal to $60^\circ$. The FE meshes of the three RVEs are shown in Figure 24. The buckling mode together with the calculated first bifurcation load factor ($\lambda_c$) for each case are shown in Figure 25. As can be seen, the same buckling mode is detected using different RVEs with close values for the first bifurcation load. However, as can be seen from Figure 26, the microscale stability contours can be different depending on the different choices of RVEs. In addition, the macroscale stability (absence of long wavelength buckling) is checked by the rank-1 convexity analysis of the homogenized tangent moduli and the results are presented in Table 8. As $B(\lambda_c) > 0$ for all cases, the rank-1 convexity of the homogenized tangent moduli is preserved and consequently there is no macroscale, that is, long wavelength, instability at the critical points associated with short wavelength buckling. As already shown in Tables 3, 4, and 6, the calculation of the homogenized tangent moduli can be slightly affected by the different choices of RVEs due to numerical errors. This influence can also be seen in the macroscale stability indicator $B(\lambda)$ calculation. Despite the small numerical differences brought by the errors in geometry and FE modeling and other approximation errors, this example demonstrates that different RVEs can be equivalently used for homogenization as well as multiscale stability analysis.

![Figure 24](image_url) FE meshes of the three different RVEs. RVE, representative volume element.
5.3 | Example-3: Hyperelastic honeycomb under different stress states

A hyperelastic honeycomb material is considered in this example with the geometry and FE model details shown in Figure 27 and matrix material properties (neo-Hookean): $\kappa = 833.33$, $\mu = 384.62$. Similar honeycomb has been examined in Reference 48. The stress driven framework is adopted to study the stability performance of the honeycomb under different stress states. Three cases are examined: (1) $\phi = \pi/2$ (uniaxial compression); (2) $\phi = \arctan(0.5)$; (3) $\phi = \pi/4$ (equi-biaxial compression). The principal stress orientation angle $\theta = 0^\circ$ and the stress amplitude (also loading parameter) $\lambda$ is increasing from zero until first bifurcation point is identified. The second case represents that the ratio of the two principle stresses is 0.5, that is, $\tau_1/\tau_2 = 0.5$. The results are shown in Figure 28. It can be seen that the three loading cases lead to different types of bifurcations—simple, double, and triple bifurcations, which is consistent with the results in Reference 48. Next, the rank-1 convexity of the homogenized tangent moduli is checked at the first bifurcation point and the results are presented in Table 9, which confirms the short wavelength type buckling as $B(\lambda_c) > 0$ for these cases.

5.4 | Example-4: Buckling mode switching in multimaterial triangular lattice

This example is used to demonstrate how the material constituents’ properties can affect the multiscale buckling behavior. A multimaterial triangular lattice-like periodic material is used with geometry and FE mesh details shown in Figure 29. Uniaxial compression along an inclined angle ($-30^\circ$) is considered with stress driven approach, that is, $\theta = -30^\circ$ and $\phi = \pi/2$ in Equations (32) and (35). The periodic material comprises two materials with material-1 plotted as red color and material-2 plotted as blue color. The parameters of material-1 are fixed as $\kappa_1 = 833.33$ and $\mu_1 = 384.62$. Three cases are
FIGURE 26  Microscale stability contours at the first bifurcation point obtained using different RVEs. RVE, representative volume element.

TABLE 8  Rank-1 convexity analysis results at first bifurcation point of the periodic material with inclined circular holes

| RVEs     | Macroscale stability indicator $B(\lambda_c)$ |
|----------|---------------------------------------------|
|          | 4.0684                                      |
|          | 4.0743                                      |
|          | 4.0748                                      |

Abbreviation: RVE, representative volume element.
considered: \((\kappa_2, \mu_2) = 0.1(\kappa_1, \mu_1), (\kappa_2, \mu_2) = (\kappa_1, \mu_1), \) and \((\kappa_2, \mu_2) = 10(\kappa_1, \mu_1)\), and the Bloch wave analysis results are shown in Figure 30. As can be seen, all the buckling wavelengths are short. However, increasing material-2 properties from \(0.1(\kappa_1, \mu_1)\) to \(10(\kappa_1, \mu_1)\) changes the microscale buckling mode from \(2 \times 2\) to \(1 \times 2\). For \((\kappa_2, \mu_2) = (\kappa_1, \mu_1)\), two aperiodic buckling modes (Figure 30(B)) are found based on the employed \(k\)-space mesh, that is, double bifurcation point. The rank-1 convexity results shown in Table 10 again confirms the short wavelength type buckling for all these cases as \(B(\lambda_c) > 0\).

### 5.5 Example-5: Highly localized buckling mode

This example intends to show a different short wavelength buckling mode, that is, a mode which has the same periodicity as the original microstructure. The geometry of the periodic material’s microstructure and the FE mesh of the RVE including one unit cell are shown in Figure 31. The matrix material follows neo-Hookean hyperelasticity with \(\kappa = 166.67\) and \(\mu = 35.71\). In this example, a strain driven loading is considered (Equation (21)) where the macroscopic deformation gradient is parameterized by \(\mathbf{F} = \lambda \cdot [1 \ 0 \ 0 \ 1]^T\) in which the loading factor \(\lambda\) is decreasing from 1, representing biaxial compression. Figure 32 shows the microscopic stability surface at the first bifurcation point \((\lambda_c = 0.9934)\) where the stability indicator \(\beta_k\) is plotted against the wavevectors \(k\) in the primitive cell in reciprocal space. As can be seen, the surface at the origin \((k_1, k_2) = (0, 0)\) is continuous, that is, the origin point is not singular, and the minimum value is indeed achieved at the origin. With the chosen \(k\) mesh, \(\beta_k\) is negative only at origin while remaining positive at other points on the surface (Figure 32(B)). This result is in contrast with that in Figure 22, where origin was a discontinuous point in the \(k\) space. This means that the buckling mode at the first bifurcation point is \(1 \times 1\) mode, that is, periodic with respect to one unit cell. The buckling mode at the first bifurcation load is plotted in Figure 33. The rank-1 convexity analysis result at \(\lambda_c, B(\lambda_c) = 5.9469\), which indicates macroscale stability.

### 5.6 Example-6: Long wavelength buckling

This example serves the purpose of demonstrating a long wavelength buckling case. The periodic material under examination is shown in Figure 34 with FE mesh of the RVE. The material’s properties follow neo-Hookean model with \(\kappa = 166.67\) and \(\mu = 35.71\). The periodic material is under a constrained compression with macroscopic deformation gradient \(\mathbf{F} = [1 \ 0 \ 0 \ \lambda]^T\) where \(\lambda\) is decreasing from one. With strain driven approach, the first bifurcation point is detected with both Bloch wave analysis and rank-1 convexity check. From stretch ratio \((\lambda)\) 0.98244 to 0.98243, both the Bloch functional indicator \(\beta(\lambda)\) in Equation (44) and the macroscopic instability indicator \(B(\lambda)\) in Equation (54) changes sign from positive to negative indicating the presence of a bifurcation point. The Bloch functional surface \(\beta_k\) at \(\lambda_c = 0.98243\) is plotted in Figure 35, while the macroscale stability curves by rank-1 convexity analysis are shown in Figure 36 for the two

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**FIGURE 27** Geometric sketch of a hyperelastic honeycomb: (A) Periodic composite; (B) unit cell; (C) FE mesh
**FIGURE 28** Microscale instability contour plots and buckling modes of the three cases under stress driven condition. Note: The principal Kirchhoff stresses \( \tau_i \) are \( \lambda_c \sin \phi \) and \( \lambda_c \cos \phi \).

**TABLE 9** Rank-1 convexity analysis results at first bifurcation point of the hyperelastic honeycomb material

| Macroscale stability indicator \( B(\lambda_c) \) | \( \phi = \pi/2 \) | \( \phi = \arctan(0.5) \) | \( \phi = \pi/4 \) |
|---|---|---|---|
| 0.2551 | 0.2559 | 0.3353 |
adjacent loading steps where \( B_a \) are the minimal values of the homogenized tangent moduli. It can be seen that long wavelength buckling can be equivalently detected from both the Bloch wave analysis and the examination of rank-1 convexity of the homogenized tangent moduli. This result is in contrast with other cases where rank-1 convexity (macrostability) is preserved at the onset of first bifurcation associated with microscale buckling with finite wavelengths.

### Example-7: Elastoplastic honeycomb under different loading orientations

The last example considers a honeycomb material with the underlying material constituent following the finite strain \( J_2 \) plasticity model with parameters \( \kappa = 17.5, \mu = 8.0, \sigma_y = 0.45, \) and \( K_p = 0.1 \) (Appendix B). Constrained compression under strain driven loading is considered with three loading orientations: \( \theta = 0^\circ \) (vertical), \( 45^\circ \) (inclined), and \( 90^\circ \) (horizontal), see Equation (82). The geometry and FE mesh details are shown in Figure 37. Same as the example in Section 3.2, the mixed u/p (9/3) element formulation is used to address the locking issue. As has been studied in Reference 38 where the honeycomb lattice is discretized using elastoplastic beam elements, the first bifurcation point depends on the loading conditions. With the 2D plane strain formulation, the Bloch stability analysis results for different macroscopic stretch orientations are given in Figure 38, where different short wavelength buckling modes are present. All are single bifurcation points. In addition, the critical load magnitude also varies according to the direction of applied loading. Figure 39 shows the deformed shapes and equivalent plastic strain (\( \alpha \)) distributions in the RVE at the first bifurcation point under different loading conditions. These results demonstrate that the inelasticity occurs before bifurcation in all these cases. Finally, the rank-1 convexity results are given in Table 11, which indicates that the macroscale stability is preserved.

**Remark:**

In contrast to the neo-Hookean hyperelastic material, the use of Hencky energy form in the finite strain \( J_2 \) plasticity is not polyconvex and may even lose ellipticity. Therefore, the rank-1 convexity of the elastoplastic model at each integration point during the loading process is numerically examined for all the examples in Sections 3.2 and 5.7 using the method in Section 4.2 with \( A \) replaced with \( \overline{A} \) at each integration point at microscale. The results show no loss of rank-1 convexity for all the considered examples.

### 6 CONCLUSIONS

In this study, a consistent computational framework is proposed for both multiscale homogenization and micro/macro stability analyses. The homogenization method is verified through hyperelastic and elastoplastic periodic materials test cases where the invariance of the homogenization results with respect to RVEs of different sizes and shapes is shown. The multiscale stability analysis with Bloch wave formulation is detailed which includes the selection of wave vector space and retrieval of the real-valued buckling mode from the complex-valued Bloch wave representations. Three methods for the resulted constrained eigenvalue problem are laid out with implementation details and the equivalence of the
\[(k_2, \mu_2) = 0.1(k_1, \mu_1): \lambda_c = 2.2464, (k_1, k_2) = (0.5, 0.5), \text{ periodic buckling mode (2\times2)}\]

\[(k_2, \mu_2) = (k_1, \mu_1): \lambda_c = 3.6160, \text{ two aperiodic buckling modes (only a small portion of buckling mode are plotted)}\]

\[(k_2, \mu_2) = 10(k_1, \mu_1): \lambda_c = 4.7109, (k_1, k_2) = (0, 0.5), \text{ periodic buckling mode (1\times2)}\]

**Figure 30**  Buckling modes of the triangular lattice obtained with different properties of material-2 (blue color)
TABLE 10  Rank-1 convexity analysis results at first bifurcation point of a triangular lattice with different properties of material-2 (blue color)

|                  | (k₂, μ₂) = 0.1(k₁, μ₁) | (k₂, μ₂) = (k₁, μ₁) | (k₂, μ₂) = 10(k₁, μ₁) |
|------------------|-------------------------|---------------------|-----------------------|
| Macroscale stability indicator $B(\lambda_c)$ | 6.7276                 | 46.7195             | 51.7206               |

**FIGURE 31** Geometric sketch of a periodic material with circular holes and inner hole cross-bars: (A) Periodic material; (B) unit cell; (C) FE mesh

**FIGURE 32** Microscale stability surface at the first bifurcation point $\lambda_c = 0.9934$

**FIGURE 33** Buckling mode (1 x 1) at the first bifurcation point $\lambda_c = 0.9934$
FIGURE 3.4 Geometric sketch of a periodic material with rotated square-shaped voids: (A) Periodic material; (B) unit cell; (C) FE mesh.

FIGURE 3.5 Microscale stability surface at the first bifurcation point $\lambda_c = 0.98243$.

FIGURE 3.6 Macroscale stability curves from rank-1 convexity analysis at before and after first bifurcation points.
**Figure 3.7** Geometric sketch of an elastoplastic honeycomb: (A) Periodic composite; (B) unit cell; (C) FE mesh

**Figure 3.8** First bifurcation loads and their corresponding buckling modes of elastoplastic honeycomb under different stretch orientations.

(a) $\theta = 0^\circ$, $\lambda_c = 0.9783$, $(k_1$, $k_2) = (0.5, 0)$

(a) $\theta = 45^\circ$, $\lambda_c = 0.9783$ $(k_1$, $k_2) = (0, 0.5)$

(a) $\theta = 90^\circ$, $\lambda_c = 0.9780$ $(k_1$, $k_2) = (0.5, 0.5)$

**Figure 3.9** Deformed shapes and equivalent plastic strain ($\alpha$) distributions of the RVE at the first bifurcation point (along the principal branch) under different stretch orientations: (A) $\theta = 0^\circ$; (B) $\theta = 45^\circ$; (C) $\theta = 90^\circ$
three methods is demonstrated. Besides, the validity of the stability analysis framework is illustrated by the equivalency of different RVEs in the stability results—first bifurcation load and the corresponding buckling mode. Several numerical examples including both hyperelastic and elastoplastic matrix materials are carried out that show various types of buckling modes—short wavelength buckling mode across over either multiple unit cells or one unit cell and long wavelength buckling mode of infinite length w.r.t. unit cell size. In accordance with the theoretical results, the numerical results also show that microscopic stability implies macroscopic stability that can be evaluated by the rank-1 convexity of the homogenized tangent moduli. Therefore, the rank-1 convexity check provides an upper bound on the critical load. In addition, the examples also show that the buckling mode can be tuned by changing the underlying matrix material properties. Moreover, in line with the previous studies, the dependence of bifurcation load on the load orientation is also demonstrated. It is important to note that the multiscale stability analysis presented in this study gives the first bifurcation load beyond which the homogenization results lose validity. To further understand the properties of the periodic material of interest after the onset of bifurcation, for example, energy absorption, band-gaps, and so forth, post-bifurcation analysis may be needed which will be the future work.

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APPENDIX A. EQUIVALENCE OF $\psi_{\min}$ AND CONSTANT TRACTION BOUNDARY CONDITION

To prove that the minimum set of kinematical admissibility in Equation (6) corresponds to constant traction boundary condition, consider the principle of multiscale virtual power with the constraints in Equation (3) enforced by the Lagrange
where $\lambda$ and $\mu$ are the Lagrange multipliers.

Assuming $\delta \tilde{F} = \delta \mu = 0$ and $\delta \lambda = 0$ in Equation (A1) gives

$$\frac{1}{V} \int_{B_0} P : \delta F dV - \lambda \int_{B_0} \delta u(X, t) dV - \mu : \left[ I + \frac{1}{V} \int_{\partial \Omega^e_0} u(X, t) \otimes N(X) dS - \tilde{F} \right] = 0 \forall \delta \mu \in \text{Lin}, \quad \delta u \in H^1(B_0), \quad \delta \lambda, \quad (A2)$$

It can be shown that

$$P : \delta F = P : \nabla X \delta u = \nabla X (P^T \cdot \delta u) - \left( \nabla X P \right) \delta u. \quad (A3)$$

Substituting Equation (A3) in Equation (A2) gives

$$\frac{1}{V} \int_{B_0} \nabla X (P^T \cdot \delta u) dV - \frac{1}{V} \int_{B_0} (\nabla X P) \cdot \delta u dV - \lambda \int_{B_0} \delta u dV - \mu : \left[ I + \frac{1}{V} \int_{\partial \Omega^e_0} \delta u \otimes N dS \right] = 0 \forall \delta u \in H^1(B_0), \quad (A4)$$

where the dependence on $X$ and $t$ is omitted for the sake of notational simplicity. Using divergence theorem on the first term in Equation (A4) gives

$$\frac{1}{V} \int_{\partial \Omega^e_0} (P.N) \cdot \delta u dS - \lambda \int_{B_0} \delta u dV - \mu : \left[ I + \frac{1}{V} \int_{\partial \Omega^e_0} \delta u \otimes N dS \right] = 0 \forall \delta u \in H^1(B_0), \quad (A5)$$

where the fact $\nabla X P = 0$ is used together with the traction-free condition on the void boundaries, that is, $P.N = 0$ on $\partial \Omega_0$.

Next, combining similar terms further gives

$$\frac{1}{V} \int_{\partial \Omega^e_0} (P.N - \mu N) \cdot \delta u dS - \lambda \int_{B_0} \delta u dV = 0 \quad \forall \delta u \in H^1(B_0) \quad (A6)$$

which, by the arbitrariness of $\delta u$, leads to the requirement that the tractions on the boundary $\partial \Omega^e_0$ should satisfy

$$t_0 = P.N = \mu N \quad \text{on} \quad \partial \Omega^e_0. \quad (A7)$$

Since the Lagrange multiplier $\mu$ is a constant second-order tensor throughout the entire domain of RVE, it is clear that the tractions on the opposite boundaries are equal valued with opposite directions. Moreover, it is straightforward to show that $\mu = \bar{P}$ by assuming $\delta u(X) = A_0 X$ in $B_0$ with $A_0 \in \text{Lin}$ using again divergence theorem on Equation (A6). Therefore, the tractions on the boundary can be expressed as

$$t_0 = \bar{P}.N \quad \text{on} \quad \partial \Omega^e_0. \quad (A8)$$

**APPENDIX B. FINITE STRAIN J2 PLASTICITY MODEL AND ITS IMPLEMENTATION**

**B.1 Finite strain J2 plasticity model**

Table B1 gives the finite strain J2 plasticity model used for the elastoplastic periodic material analyses. The multiplicative split of the deformation gradient is assumed, that is, $F = F^e F^p$ where $F^e$ and $F^p$ represent the elastic and plastic part of the deformation gradient, respectively. Linear isotropic hardening is considered.
TABLE B1 Finite strain $J_2$ plasticity model

Yield function: \( \phi(\tau, \alpha) = \|\tau_{\text{dev}}\| - \sqrt{\frac{2}{3}} \zeta(\alpha), \) \hspace{1cm} (B1)

where

\[ \tau_{\text{dev}} = \mathbb{P}_{\text{dev}}^\tau : \tau \quad \text{with} \quad (\mathbb{P}_{\text{dev}}^\tau)_{ij} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) - \delta_{ij} \delta_{kl}, \] \hspace{1cm} (B2)

\[ \zeta(\alpha) = \sigma_y + Kp \alpha. \] \hspace{1cm} (B3)

Free energy: \( \psi^e(\mathbf{b}^e) = \psi_{\text{vol}}^e(J^e) + \psi_{\text{iso}}^e(\mathbf{b}^e), \) \hspace{1cm} (B4)

\[ \psi_{\text{vol}}^e(J^e) = \frac{1}{2} \kappa (\ln J^e)^2 = \frac{1}{2} \kappa (\epsilon_1^e + \epsilon_2^e + \epsilon_3^e)^2, \] \hspace{1cm} (B5)

\[ \psi_{\text{iso}}^e(\mathbf{b}^e) = \frac{\mu}{4} I : (\ln \mathbf{b}^e)^2, \] \hspace{1cm} (B6)

where

\[ J^e = \sqrt{\det \mathbf{b}^e} = \lambda_1^e \lambda_2^e \lambda_3^e, \] \hspace{1cm} (B7)

\[ \epsilon_i^e = \ln \lambda_i^e, \quad i = 1, 2, 3, \] \hspace{1cm} (B8)

\[ \mathbf{b}^e = J^{-1/3} \mathbf{b}^e, \] \hspace{1cm} (B9)

\[ \mathbf{b}^e = F e F^T. \] \hspace{1cm} (B10)

Isotropic elasticity: \( \tau = 2 \frac{\partial \psi^e}{\partial \mathbf{b}^e} \mathbf{b}^e. \) \hspace{1cm} (B11)

Flow rules: \( \frac{1}{2} \mathcal{L}_\epsilon(\mathbf{b}^e) \cdot \mathbf{b}^{e-1} = \frac{\gamma}{\tau} \frac{\partial \phi}{\partial \tau} \quad \Rightarrow \quad \mathbf{C}^e = -2 \gamma F^{-1} \frac{\partial \phi}{\partial \tau} F \mathbf{C}^e, \) \hspace{1cm} (B12)

\[ \dot{\alpha} = -\gamma \frac{\partial \phi}{\partial \zeta} = \sqrt{\frac{2}{3}} \gamma \] \hspace{1cm} (B13)

where

\[ \mathbf{C}^e \overset{\text{def}}{=} \mathbf{C}^{e-1}, \quad \mathbf{C}^e = F^T \mathbf{F}. \] \hspace{1cm} (B14)

KKT conditions: \( \gamma \geq 0, \quad \phi \leq 0, \quad \gamma \phi = 0. \) \hspace{1cm} (B15)

Consistency condition: \( \gamma \dot{\phi} = 0. \) \hspace{1cm} (B16)

Note: \( \tau \)—Kirchhoff stress tensor; \( \mathbf{b}^e \), elastic Finger tensor; \( \lambda_i^e \), \( i \)-th elastic principal stretch; \( \alpha \), equivalent plastic strain; \( \sigma_y \), initial yield stress; \( Kp \), hardening modulus; \( \kappa, \mu \), bulk and shear modulus.

B.2 Implementation details

For the numerical implementation of the model, in the context of the strain-driven finite element formulation, given data at an integration point: \( F_k, \mathbf{C}_k \), and \( \alpha_k \) at previous step \( k \), and \( F \) at current step \( k + 1 \), the goal is to find the unknown variables: \( \tau, \mathbf{C}^e, \) and \( \alpha \) and the consistent tangent moduli at the current step. Note that the subscript \( k + 1 \) for the current step is omitted for the sake of clarity.

In the implementation, elastic step assumption is first examined assuming no plastic flow, that is, \( \mathbf{C}^e = \mathbf{C}^{e-1}_k, \mathbf{b}^e = \mathbf{b}^{e-1}_k \), and \( \alpha = \alpha_k \), and the stress \( \tau \) can be accordingly computed by Equation (B11). The elastic assumption is then checked by examining the criterion \( \phi(\tau, \alpha) \leq 0 \). If yes, all the calculated stress and updated internal variables are the true values. If no
(i.e., $\phi > 0$), the elastic assumption is wrong and there is nonzero plastic flow. Then the computations given in Sections B.2.1–B.2.2 are needed to compute the stress and internal variables. The computation of consistent tangent moduli is given in Section B.2.3.

### B.2.1 Integration of rate equations

The flow rule given in Equation (B12) is integrated using the exponential integrator as

$$C^i = \exp \left( -2\gamma \left( F^{-1} \frac{\partial \phi}{\partial \tau} F \right) \Delta t \right) \cdot C_k^i$$

(B17)

which, by defining $b^{e\text{tr}} = F^{e\text{tr}} F^{e\text{tr}}^T$ (or equivalently $b^{e\text{tr}} = F C_k^i F^T$) with $F^{e\text{tr}} = F_k^e F_k^e$ and $F_k = F_k F_k^{-1}$, can be rewritten as

$$b^e = \exp(-2\Delta \gamma \tilde{n}), b^{e\text{tr}},$$

(B18)

where $\Delta \gamma = \gamma \Delta t$ and $\tilde{n} \overset{\text{def}}{=} \tau_{\text{dev}}/\|\tau_{\text{dev}}\| = \partial \phi / \partial \tau$ are applied.

Due to isotropy, the tensors $\tau$, $b^e$, $b^{e\text{tr}}$, and $\tilde{n}$ are coaxial, see Equation (B11). Therefore, it is possible to express the evolution Equation (B18) in the principal space. Taking the logarithm of Equation (B18), that is,

$$e^e = e^{e\text{tr}} - \Delta \gamma \tilde{n}$$

(B19)

with $e^e = \frac{1}{2} \ln b^e$ and $e^{e\text{tr}} = \frac{1}{2} \ln b^{e\text{tr}}$, the principle space discretization gives

$$\sum_{a=1}^{3} (e^e_a + \Delta \gamma \tilde{n}_a) n^a \otimes n^a = \sum_{a=1}^{3} e^{e\text{tr}}_a n_a^{e\text{tr}} \otimes n_a^{e\text{tr}}$$

(B20)

and thus leads to

$$[e^e] = [e^{e\text{tr}}] - \Delta \gamma [\tilde{n}]$$

with $[e^e] = \begin{bmatrix} e^e_1 \\ e^e_2 \\ e^e_3 \end{bmatrix}$, $[e^{e\text{tr}}] = \begin{bmatrix} e^{e\text{tr}}_1 \\ e^{e\text{tr}}_2 \\ e^{e\text{tr}}_3 \end{bmatrix}$, $[\tilde{n}] = \begin{bmatrix} \tilde{n}_1 \\ \tilde{n}_2 \\ \tilde{n}_3 \end{bmatrix}$

(B21)

and

$$n_a = n_a^{e\text{tr}}, \quad a = 1, 2, 3,$$

(B22)

where $e^{e\text{tr}}_a$ and $\tilde{n}_a$ ($a = 1, 2, 3$) are the eigenvalues of tensors $e^{e\text{tr}}$ and $\tilde{n}$, respectively. Here $n_a$ are the eigenvectors of $\tilde{n}$ (also $\tau$, $b^e$, and $e^e$), and $n_a^{e\text{tr}}$ are the eigenvectors of $e^{e\text{tr}}$ (also $b^{e\text{tr}}$).

The integration of Equation (B13) is carried out using backward Euler scheme as

$$\alpha = \alpha_k + \sqrt{\frac{2}{3}} \Delta \gamma.$$  

(B23)

### B.2.2 Solution of stress and internal variables

The computation of the stress tensor $\tau$ and internal variables $C^i$ and $\alpha$ can be simplified down to the computation of the scalar $\Delta \gamma$ through a nonlinear equation. To see this, the calculation of principle stresses vectors $[\tau_{\text{vol}}]$ and $[\tau_{\text{dev}}]$ are first derived from Equations (B11) and (B4)–(B6) as

$$[\tau_{\text{vol}}] = \frac{\partial \psi_{\text{vol}}}{\partial e^e} = 3k[\tilde{P}_{\text{vol}}][\epsilon^e],$$

(B24)

$$[\tau_{\text{dev}}] = \frac{\partial \psi_{\text{dev}}}{\partial e^e} = 2\mu[\tilde{P}_{\text{dev}}][\epsilon^e],$$

(B25)
where

\[
[\mathbb{P}_{\text{vol}}] = \frac{1}{3} [1][1]^T = \frac{1}{3} \begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{bmatrix},
\]

\[
[\mathbb{P}_{\text{dev}}] = [I] - \frac{1}{3} [1][1]^T = \begin{bmatrix}
\frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\
-\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\
-\frac{1}{3} & -\frac{1}{3} & \frac{2}{3}
\end{bmatrix}.
\]

(B26)

Next, the substitution of Equation (B21) into Equation (B25) gives

\[
[\tau_{\text{dev}}] = [\tau_{\text{dev}}^{\text{tr}}] - 2\mu \Delta \gamma [\hat{n}] 
\]

or \( \tau_d - r_d^{\text{tr}} + 2\mu \Delta \gamma = 0 \). (B27)

where \([\tau_{\text{dev}}^{\text{tr}}]\) = 2\mu[\mathbb{P}_{\text{dev}}][\varepsilon^{\text{tr}}], \([\tau_{\text{dev}}] = r_d[\hat{n}]\) and \([\tau_{\text{dev}}^{\text{tr}}] = r_d^{\text{tr}}[\hat{n}]^{\text{tr}}\) are considered. Remember that \([\hat{n}] = [\hat{n}]^{\text{tr}}\) from Equation (B22) and

\[
[\hat{n}]^{\text{tr}} = \frac{[\tau_{\text{dev}}^{\text{tr}}]}{||[\tau_{\text{dev}}]||} = \frac{[\mathbb{P}_{\text{dev}}][\varepsilon^{\text{tr}}]}{\sqrt{[\varepsilon^{\text{tr}}]^T [\mathbb{P}_{\text{dev}}][\varepsilon^{\text{tr}}]}}.
\]

(B28)

Hence, it is obvious that \(\Delta \gamma\) is the only unknown variable in the equation \(\phi(\tau(\Delta \gamma), a(\Delta \gamma)) = 0\) and can be solved using NR method. To be complete, the resulted nonlinear equation is given below

\[
R(\Delta \gamma) = r_d - 2\mu \Delta \gamma - \sqrt{\frac{2}{3}} \left[ \sigma + K^P \left( \alpha + \sqrt{\frac{2}{3}} \Delta \gamma \right) \right] = 0
\]

(B29)

with the Jacobian calculated as

\[
\frac{dR(\Delta \gamma)}{d\Delta \gamma} = -2\mu - \frac{2}{3} K^P.
\]

(B30)

After finding the solution of \(\Delta \gamma\), both the stress tensor \(\tau\) and internal variables \((C, a)\) can be updated accordingly, see Equations (B21)–(B28). The first PK stress \(P\) can be simply computed by \(P = \tau F^{-T}\).

**B.2.3 Consistent tangent moduli**

The consistent tangent moduli \(A = \partial P / \partial F\) is needed for obtaining asymptotic quadratic convergence in the global NR solver. For notational convenience, in addition to standard tensor notations, the below nonstandard tensor notations are utilized in the following derivations.

\[
(A \boxtimes B)_{ijkl} \overset{\text{def}}{=} A_{il} B_{jk},
\]

\[
(A \boxplus B)_{ijkl} \overset{\text{def}}{=} A_{ik} B_{jl},
\]

(B31)

where \(A\) and \(B\) are any second-order tensors.

The tangent moduli \(A\) is calculated by the pull-back of tensor \(a\) as

\[
A_{ijkl} = J F_{jm}^{-1} \varepsilon_{ikm} b_{ln} F_{ln}^{-1}
\]

with \(J a = \frac{\partial \tau}{\partial \varepsilon^{\text{tr}}} : (I \boxtimes b^{\text{tr}} + b^{\text{tr}} \boxplus I) - \tau \boxplus I\). (B32)

where the derivative \(\partial \tau / \partial b^{\text{tr}}\) is computed using chain rule.
\[
\frac{\partial \tau}{\partial \varepsilon^e} = \frac{\partial \tau}{\partial \varepsilon^p} \cdot \frac{\partial \varepsilon^p}{\partial \varepsilon^e}.
\] (B33)

Since the tensors \(\tau, \varepsilon^e,\) and \(\varepsilon^p\) are coaxial, following the procedures given in the Appendix A in Reference 63, the calculation of the terms \(\partial \tau / \partial \varepsilon^p\) and \(\partial \varepsilon^p / \partial \varepsilon^e\) can be carried out in the eigen space and requires only \(\partial [\tau] / \partial [\varepsilon^p]\) and \(\partial [\varepsilon^p] / \partial [\varepsilon^e]\).

The computation of \(\partial [\varepsilon^p] / \partial [\varepsilon^e]\) is trivial and is given by

\[
\frac{\partial [\varepsilon^p]}{\partial [\varepsilon^e]} = \begin{bmatrix}
\frac{1}{2 \lambda^e} & 0 & 0 \\
0 & \frac{1}{2 \lambda^e} & 0 \\
0 & 0 & \frac{1}{2 \lambda^e}
\end{bmatrix}.
\] (B34)

The computation of \(\partial [\tau] / \partial [\varepsilon^p]\) is computed differently depending on whether it is elastic step or plastic step.

**Elastic step**

For elastic step, from Equations (B24) and (B25), it is straightforward that

\[
\frac{\partial [\tau]}{\partial [\varepsilon^p]} = 3 \kappa [P_{\text{vol}}] + 2 \mu [P_{\text{dev}}].
\] (B35)

**Plastic step**

For plastic step, the required derivative \(\partial [\tau] / \partial [\varepsilon^p]\) is calculated as

\[
\frac{\partial [\tau]}{\partial [\varepsilon^p]} = \frac{\partial [\tau_{\text{vol}}]}{\partial [\varepsilon^p]} + \frac{\partial [\tau_d]}{\partial [\varepsilon^p]} + \frac{\partial [\widetilde{n}_{\text{tr}}]}{\partial [\varepsilon^p]}.
\] (B36)

Analogous to Equation (B27), the substitution of Equations (B21–(B24) gives

\[
[r_{\text{vol}}] = 3 \kappa [P_{\text{vol}}] ([\varepsilon^p] - \Delta \gamma [\widetilde{n}]) = [r_{\text{vol}}]^{\text{tr}} \quad \text{with} \quad [r_{\text{vol}}]^{\text{tr}} = 3 \kappa [P_{\text{vol}}][\varepsilon^p]
\] (B37)

and thus

\[
\frac{\partial [r_{\text{vol}}]}{\partial [\varepsilon^p]} = 3 \kappa [P_{\text{vol}}].
\] (B38)

The term \(\partial \tau_d / \partial [\varepsilon^p]\) can be computed through chain rule, according to Equation (B27)_2, as

\[
\frac{\partial \tau_d}{\partial [\varepsilon^p]} = \frac{\partial \tau_d^{\text{tr}}}{\partial [\varepsilon^p]} - 2 \mu \frac{\partial \Delta \gamma}{\partial [\varepsilon^p]}.
\] (B39)

Taking the derivative w.r.t. \([\varepsilon^p]\) on both sides of Equation (B29) gives

\[
\frac{d \Delta \gamma}{d [\varepsilon^p]} = \frac{1}{2 \mu + \frac{2}{3} K_p} \frac{\partial \tau_d^{\text{tr}}}{d [\varepsilon^p]},
\] (B40)

and the remaining derivatives that need to be calculated are \(\partial \tau_d^{\text{tr}} / \partial [\varepsilon^p]\) and \(\partial [\widetilde{n}_{\text{tr}}] / \partial [\varepsilon^p]\) which are given as

\[
\frac{\partial \tau_d^{\text{tr}}}{\partial [\varepsilon^p]} = \frac{2 \mu [P_{\text{dev}}][\varepsilon^p]}{\sqrt{[\varepsilon^p]^T [P_{\text{dev}}][\varepsilon^p]}},
\] (B41)
\[
\frac{\partial [n]^{tr}}{\partial [\epsilon^{dev}]} = \frac{[P_{dev}]}{\sqrt{[\epsilon^{dev}]^T [P_{dev}] [\epsilon^{dev}]} - \frac{[P_{dev}] [\epsilon^{dev}][\epsilon^{dev}]^T [P_{dev}]}{([\epsilon^{dev}]^T [P_{dev}] [\epsilon^{dev}])^{\frac{3}{2}}},
\]

(B42)

where the expression \( \tau_d^{tr} = 2\mu \sqrt{[\epsilon^{dev}]^T [P_{dev}] [\epsilon^{dev}]} \) is used.