Numerical homogenization of dual-phase steel by nonlinear conjugate gradient method

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Abstract

A numerical method is proposed to solve a cell problem for numerical homogenization of composite material, all of whose phases are homogeneous isotropic and whose deformations follow the elastoplastic constitutive law of Hencky's total strain theory.

1 Introduction

We propose a numerical method for solving a cell problem for homogenization of a nonlinear elastic system that is derived from an elasto-plastic constitutive relation of the total strain theory. The cell problem is to find a deformation u on the unit cell $Y = [0,1]^3$ subjected to a macroscopic strain $\boldsymbol{E}$. The governing equation of the cell problem are;

$$\begin{cases} \sum_{j=1}^{3} \partial_j \sigma_{ij}(x) = 0 \\ \sigma_{ij}(x) = \frac{\partial}{\partial \epsilon_{ij}} W(x, \epsilon + \boldsymbol{E}) \\ \epsilon_{ij} = \frac{1}{2}\left(\partial_j u_i + \partial_i u_j\right) \end{cases}$$

where W is the strain energy density function of the nonlinear system. The solution of the cell problem is used to evaluate the macroscopic response $\boldsymbol{\Sigma}$ of the material to the macroscopic strain $\boldsymbol{E}$:

$$\boldsymbol{\Sigma}_{ij} = \int_Y \sigma_{ij}(x) dx.$$

The cell problem is equivalent to the minimization problem over deformations u satisfying the periodic boundary condition

$$\min_u \int_Y W(x, \epsilon(u) + \boldsymbol{E}) dx. \tag{1}$$

In this paper, we develop an efficient algorithm for solving the minimization problem (1).

1.1 The elastoplastic constitutive law and the strain energy function

We recall the elasto-plastic model of the total-strain theory [3, 4]. First, we list some of the notations; E and ν denote Young's modulus and the Poisson ratio, respectively. μ and λ represent the shear modulus and Lamé's first parameter, respectively; $\mu = \frac{E}{2(1+\nu)}, \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$. $K = \lambda + \frac{2}{3}\mu$ is the bulk modulus. All stresses σ and strains ϵ considered in this study are true stress (Cauchy stress) and true strain. The deviatoric strain ϵ'_{ij} and deviatoric stress σ'_{ij} are defined by

$$\epsilon'_{ij} = \epsilon_{ij} - \frac{1}{3}\,\mathrm{tr}(\epsilon)\delta_{ij}, \quad \sigma'_{ij} = \sigma_{ij} - \frac{1}{3}\,\mathrm{tr}(\sigma)\delta_{ij}.$$

$\|t\| = \sqrt{\sum_{i,j=1}^{3} t_{ij}^2}$ denotes the norm of a second order tensor $t = \{t_{ij}\}_{i,j=1,2,3}$. $|\sigma| = \sqrt{\frac{3}{2}}\|\sigma'\|$ is the von Mises equivalent stress, and $|\epsilon| = \sqrt{\frac{2}{3}}\|\epsilon'\|$ is the von Mises equivalent strain.

The elasto-plastic model is composed of three basic building blocks. First, the total strain is the sum of elastic and plastic strain.

$$\epsilon_{ij} = \epsilon^e_{ij} + \epsilon^p_{ij}. \tag{2}$$

Second, a Hookean-type constitutive relation is assumed

$$\sigma_{ij} = 2\mu(\epsilon^e)'_{ij} + K\,\mathrm{tr}(\epsilon^e)\delta_{ij}, \tag{3}$$

where $(\epsilon^e)'$ is the deviatoric part of elastic stress. Finally, the plastic component of strain is proportional to deviatoric stress.

$$\epsilon^p_{ij} = \frac{3\eta}{2|\sigma|}\sigma'_{ij}, \qquad \eta \in f(|\sigma|). \tag{4}$$

where $f(s)$ is the nonnegative (possibly single-valued) function for $s \geq 0$. For example, the elastic-perfectly plastic model can be obtained by the following function:

$$f(s) = \begin{cases} 0 & 0 \leq s < \sigma_y \\ [0,\infty] & s = \sigma_y \\ \infty & s > \sigma_y. \end{cases}$$

1.2 Nonlinear elastic system

It is well known that the elasto-plastic constitutive relation can be represented as a nonlinear elastic system [5]. We will describe the detail here for the sake of completeness.

From the constitutive laws (2), (3), and (4), we obtain the equation

$$\epsilon_{ij} = \left(\frac{1}{2\mu} + \frac{3\eta}{2|\sigma|}\right)\sigma'_{ij} + \frac{1}{9K}\operatorname{tr}(\sigma)\delta_{ij}, \qquad \eta \in f(|\sigma|).$$

Inverting this relation leads to

$$\sigma_{ij} = \frac{2\mu|\sigma|}{|\sigma| + 3\mu\eta}\epsilon'_{ij} + K\operatorname{tr}(\epsilon)\delta_{ij}, \qquad \eta \in f(|\sigma|). \tag{5}$$

The deviatoric part of the stress in (5) is

$$\sigma'_{ij} = \frac{2\mu|\sigma|}{|\sigma| + 3\mu\eta}\epsilon'_{ij}, \qquad \eta \in f(|\sigma|),$$

which yields $\|\sigma'\| = \frac{2\mu|\sigma|}{|\sigma|+3\mu\eta}\|\epsilon'\|$ or equivalently $|\sigma| = \frac{3\mu|\sigma|}{|\sigma|+3\mu\eta}|\epsilon|$. Therefore we have

$$\frac{|\sigma|}{3\mu} + \eta = |\epsilon|, \qquad \eta \in f(|\sigma|).$$

Now we assume that, for any $t \geq 0$, there exists a unique pair of nonnegative real numbers (s, p) that satisfies the inclusion

$$\frac{s}{3\mu} + p = t, \qquad p \in f(s). \tag{6}$$

We denote the solution of the inclusion by $(s(t), p(t))$.

Let us assume that the strain ϵ is given. Define σ_{ij}, ϵ^e_{ij} and ϵ^p_{ij} by

$$\begin{aligned} \sigma_{ij} &= \frac{2\mu s(|\epsilon|)}{s(|\epsilon|) + 3\mu p(|\epsilon|)}\epsilon'_{ij} + K\operatorname{tr}(\epsilon)\delta_{ij}, \\ \epsilon^e_{ij} &= \frac{1}{2\mu}\sigma'_{ij} + \frac{1}{9K}\operatorname{tr}(\sigma)\delta_{ij} \\ \epsilon^p_{ij} &= \frac{3p(|\epsilon|)}{2s(|\epsilon|)}\sigma'_{ij}. \end{aligned} \tag{7}$$

We show that $\sigma, \epsilon^e, \epsilon^p$ satisfies the constitutive relation (2), (3) and (4).

Since, $\sigma'_{ij} = \frac{2\mu s(|\epsilon|)}{s(|\epsilon|)+3\mu p(|\epsilon|)}\epsilon'_{ij}$ and $\operatorname{tr}(\sigma) = (3\lambda + 2\mu)\operatorname{tr}(\epsilon)$, we obtain

$$\epsilon_{ij} = \epsilon'_{ij} + \frac{1}{3}\operatorname{tr}(\epsilon)\delta_{ij} = \left(\frac{1}{2\mu} + \frac{3p(|\epsilon|)}{2s(|\epsilon|)}\right)\sigma'_{ij} + \frac{1}{9K}\operatorname{tr}(\sigma)\delta_{ij} = \epsilon^e_{ij} + \epsilon^p_{ij},$$

and

$$|\sigma| = \sqrt{\frac{3}{2}}\|\sigma'\| = \sqrt{\frac{3}{2}}\frac{2\mu s(|\epsilon|)}{s(|\epsilon|) + 3\mu p(|\epsilon|)}\|\epsilon'\| = s(|\epsilon|).$$

Based on the definition of $p(|\epsilon|)$, we have $p(|\epsilon|) \in f(s(|\epsilon|)) = f(|\sigma|)$. Therefore the constitutive relation (2), (3) and (4) is equivalent to the nonlinear elastic system (7).

Let $g(\xi) = \frac{p(\sqrt{\xi})}{\sqrt{\xi}}$ be the degree of plasticity [6]. The nonlinear elastic system (7) can also be represented as

$$\sigma_{ij} = 2\mu\left(1 - \frac{p(|\epsilon|)}{|\epsilon|}\right)\epsilon'_{ij} + K\,\mathrm{tr}(\epsilon)\delta_{ij} = 2\mu(1 - g(|\epsilon|^2))\epsilon_{ij} + \left(\lambda + \frac{2}{3}g(|\epsilon|^2)\right)\mathrm{tr}(\epsilon)\delta_{ij} \tag{8}$$

because

$$\sigma'_{ij} = 2\mu\frac{s(|\epsilon|)}{s(|\epsilon|) + 3\mu p(|\epsilon|)}\epsilon'_{ij} = 2\mu\frac{3\mu|\epsilon| - 3\mu p(|\epsilon|)}{3\mu|\epsilon|}\epsilon'_{ij} = 2\mu\left(1 - \frac{p(|\epsilon|)}{|\epsilon|}\right)\epsilon'_{ij}.$$

The constitutive relation is reduced to Hook's law when $p(|\epsilon|) = 0$:

$$\sigma_{ij} = 2\mu\epsilon_{ij} + \lambda\,\mathrm{tr}(\epsilon)\delta_{ij}.$$

Remark 1. *The existence of the unique solution of the inclusion* (6) *is guaranteed if f is maximally monotone by Minty theorem [2, Theorem 3.5.8].*

The strain energy density function for the nonlinear elastic system (8), i.e., the function W such that $\sigma_{ij} = \frac{\partial W}{\partial \epsilon_{ij}}$, is given as follows

$$W(\epsilon) = \mu\|\epsilon\|^2 + \frac{\lambda}{2}\,\mathrm{tr}(\epsilon)^2 - 3\mu\int_0^{|\epsilon|} p(\tau)d\tau.$$

Example
At the end of this section, we give one example of the elastoplastic model. A material which deforms plastically without hardening even after reaching yield stress is modeled as the elastic-perfectly plastic material: The stress-strain curve for the uniaxial tension test is given by

$$\sigma = \begin{cases} E\epsilon & 0 \le \epsilon \le \frac{\sigma_y}{E}, \\ \sigma_y & \frac{\sigma_y}{E} \le \epsilon. \end{cases}$$

where σ_y is the yield stress. The flow stress-strain curve of this model is given by

$$f(s) = \begin{cases} 0 & 0 \le s < \sigma_y \\ [0,\infty] & s = \sigma_y \\ \infty & s > \sigma_y. \end{cases}$$

It is easy to see that the unique solution $(s(t), p(t))$ of the inclusion $s + 3\mu p = 3\mu t, p \in f(s)$ for $t \ge 0$ is given as

$$(s(t), p(t)) = \begin{cases} (3\mu t, 0) & 0 \le t < \frac{\sigma_y}{3\mu} \\ (\sigma_y, t - \frac{\sigma_y}{3\mu}) & \frac{\sigma_y}{3\mu} \le t, \end{cases}$$

hence, the constitutive relation for the elastic-perfectly plastic is

$$\sigma_{ij} = \begin{cases} 2\mu\epsilon'_{ij} + K\,\mathrm{tr}(\epsilon)\delta_{ij} & 0 \le |\epsilon| < \frac{\sigma_y}{3\mu}, \\ \frac{2\sigma_y}{3|\epsilon|}\epsilon'_{ij} + K\,\mathrm{tr}(\epsilon)\delta_{ij} & \frac{\sigma_y}{3\mu} \le |\epsilon|. \end{cases}$$

We obtain the strain energy density function that is similar, but not identical, to the density function presented in the monograph [1, Chapter 14]:

$$W(\epsilon) = \begin{cases} 2\mu\|\epsilon\|^2 + \lambda\,\mathrm{tr}(\epsilon)^2 & 0 \le |\epsilon| < \frac{\sigma_y}{3\mu}, \\ \sigma_y|\epsilon|^2 - \frac{\sigma_y^2}{6\mu} + \frac{K}{2}\,\mathrm{tr}(\epsilon)^2 & \frac{\sigma_y}{3\mu} \le |\epsilon| \end{cases}$$

2 Nonlinear PCG for the cell problem

Let $W(x,\epsilon)$ be the strain density function that depends on the location x in the unit cell Y.

$$W(x,\epsilon) = \mu(x)\|\epsilon\|^2 + \frac{\lambda(x)}{2}\,\mathrm{tr}(\epsilon)^2 - 3\mu(x)\int_0^{|\epsilon|} p(x,\tau)d\tau$$

Here $(s(x,\tau), p(x,\tau))$ is the unique solution (s,p) of the inclusion

$$s + 3\mu(x)p = 3\mu(x)\tau, \quad p \in f(x,s).$$

Let J be the total energy on the space

$$H^1_\sharp(Y,\mathbf{R}^3) = \{u \in H^1(Y,\mathbf{R}^3) \mid u \text{ is } Y\text{-periodic and } \int_Y u_i(y)dy = 0, i = 1,2,3\}$$

subject to the macroscopic strain $\boldsymbol{E}$

$$J(u) := \int_Y W(x, \epsilon(u) + \boldsymbol{E})dx.$$

The directional derivative of $J(u)$ in a direction d for the nonlinear elastic system (8) is given as

$$\langle J'(u), d\rangle := \frac{d}{dt}J(u+td)|_{t=0} = \int_Y \left(2\tilde{\mu}(x)\boldsymbol{e}_{ij}\epsilon(d)_{ij} + \tilde{\lambda}(x)\,\mathrm{tr}(\boldsymbol{e})\,\mathrm{tr}(\epsilon(d))\right)dx$$

where we use notations:

$$\boldsymbol{e} = \epsilon(u) + \boldsymbol{E}, \quad \tilde{\lambda}(x) = \lambda(x) + \frac{2}{3}\mu(x)g(|\boldsymbol{e}|^2), \quad \tilde{\mu}(x) = \mu(x)(1 - g(|\boldsymbol{e}|^2)). \quad (9)$$

The steepest "ascent" direction $g = (g^1, g^2, g^3)$ in the distribution sense is given by

$$\begin{cases} g^1 &= (\partial_x)^*\left\{2\tilde{\mu}(x)\boldsymbol{e}_{11} + \tilde{\lambda}(x)\,\mathrm{tr}(\boldsymbol{e})\right\} + (\partial_y)^*(2\tilde{\mu}(x)\boldsymbol{e}_{12}) + (\partial_z)^*(2\tilde{\mu}(x)\boldsymbol{e}_{13}), \\ g^2 &= (\partial_x)^*(2\tilde{\mu}(x)\boldsymbol{e}_{12}) + (\partial_y)^*\left\{2\tilde{\mu}(x)\boldsymbol{e}_{22} + \tilde{\lambda}(x)\,\mathrm{tr}(\boldsymbol{e})\right\} + (\partial_z)^*(2\tilde{\mu}(x)\boldsymbol{e}_{23}), \\ g^3 &= (\partial_x)^*(2\tilde{\mu}(x)\boldsymbol{e}_{13}) + (\partial_y)^*(2\tilde{\mu}(x)\boldsymbol{e}_{23}) + (\partial_z)^*\left\{2\tilde{\mu}(x)\boldsymbol{e}_{33} + \tilde{\lambda}(x)\,\mathrm{tr}(\boldsymbol{e})\right\} \end{cases} \quad (10)$$

Here $\partial_i^* = -\partial_i$ for $i = x, y, z$.

Problem formulation. Let $\boldsymbol{E}$ be a prescribed macroscopic strain. Our object is to find the deformation $u^* \in H^1_\sharp(Y, \mathbf{R}^3)$ on the unit cell $Y = [0,1]^3$:

$$u^* = \arg \min_{u \in H^1_\sharp(Y,\mathbf{R}^3)} J(u)$$

and the macroscopic response stress $\boldsymbol{\Sigma}$

$$\boldsymbol{\Sigma}_{ij} = \int_Y \sigma_{ij}(x)dx = \int_Y (2\mu(x)(1-g(|\boldsymbol{e}^*|^2))\boldsymbol{e}^*_{ij} + \left(\lambda(x) + \frac{2\mu(x)}{3} g(|\boldsymbol{e}^*|^2)\right) \operatorname{tr}(\boldsymbol{e}^*)\delta_{ij})dx \tag{11}$$

where $\boldsymbol{e}^* = \epsilon(u^*) + \boldsymbol{E}$.

Discretization. We discretize the total energy function by a standard staggered-grid finite-difference method. The implementation details are omitted.

Algorithm. We conisder the nonlinear preconditioned conjugate gradient (PCG) algorithm for the minimization problem of J. The PCG requires a variable metric at any u to define the Riesz representation of the derivative $J'(u)$ associated with the metric. We introduce an inner product defined at u ([6])

$$a(u; v, w) := \int_Y \left(2\tilde{\mu}(x)\epsilon(v)_{ij}\epsilon(w)_{ij} + \tilde{\lambda}(x) \operatorname{tr}(\epsilon(v)) \operatorname{tr}(\epsilon(w))\right) dx$$

where $\tilde{\mu}, \tilde{\lambda}$ are defined by (9). With this notation, we have

$$a(u + \boldsymbol{E}x; u + \boldsymbol{E}x, d) = \langle J'(u), d\rangle$$

for $x \in Y$. Here $(\boldsymbol{E}x)_i = \sum_{j=1}^3 \boldsymbol{E}_{ij}x_j$. The Riesz representation of $J'(u)$ is the solution z of the variational problem

$$a(u + \boldsymbol{E}x; z, v) = \langle J'(u), v\rangle \qquad \forall v \in H^1_\sharp(Y, \mathbf{R}^3)$$

The optimality condition for z is a linear system with the variable coefficients $\tilde{\mu}(x), \tilde{\lambda}(x)$. To reduce the computational costs for solving the linear system, we replace the variational problem with the following one:

$$\bar{a}(u + \boldsymbol{E}x; z, v) = \langle J'(u), v\rangle \qquad \forall v \in H^1_\sharp(Y, \mathbf{R}^3) \tag{12}$$

where

$$\bar{a}(u + \boldsymbol{E}x; z, v) = \int_Y \left(2\bar{\mu}\epsilon(v)_{ij}\epsilon(w)_{ij} + \bar{\lambda} \operatorname{tr}(\epsilon(v)) \operatorname{tr}(\epsilon(w))\right) dx$$

$$\bar{\mu} := \int_Y \tilde{\mu}(x)dx, \quad \bar{\lambda} := \int_Y \tilde{\lambda}(x)dx$$

The optimality system for the variational problem (12) is linear system with constant coefficients, and the solution can be obtained in the frequency domain by Fourier transformation.

We present the nonlinear PCG for the solution of the minimization problem $\min_{u \in H^1_\sharp(Y,\mathbf{R}^3)} J(u)$. We assume that all quantities are appropriately discretized, but describe the numerical algorithm using the same symbols for operations on continuous quantities.

Algorithm 1: Nonlinear PCG for the solution of $\min_{u \in H^1_\sharp(Y,\mathbf{R}^3)} J(u)$
Input: macroscopic strain $\boldsymbol{E}$
Initialization:
Start with an initial guess u^0 and compute the steepest ascent g^0 of J at u_0 by (10)
Solve the variational problem (12) for z^0.
Set the initial search direction $d^0 = -z^0$
Main loop:
for $k = 0, 1, 2, \dots$ **do**
Compute the step length $s = \arg\min_{t>0} J(u^k + td^k)$ and update $u^{k+1} = u^k + sd^k$
Compute the steepest ascent direction $g^{k+1} = (g_1^{k+1}, g_2^{k+1}, g_3^{k+1})$ by (10)
Solve the variational problem (12) for z^{k+1}
Compute the search direction $d^{k+1} = -z^{k+1} + \beta d^k$ for given $\beta > 0$
end for
Output: The macroscopic stress $\boldsymbol{\Sigma}$ by (11)

Remark 2. *The parameter β is given as, for instance*

$$\beta = \frac{(g_1^{k+1} - g_1^k, z_1^{k+1}) + (g_2^{k+1} - g_2^k, z_2^{k+1}) + (g_3^{k+1} - g_3^k, z_3^{k+1})}{(g_1^k, z_1^k) + (g_2^k, z_2^k) + (g_3^k, z_3^k)}$$

where $(f, g) = \int_Y f(x)g(x)dx$. See [7] for the discussion of the choice of β.

2.1 PCG for uniaxial tension tests

We will denote the space of 3×3 symmetric matrices by M_S. Define $J\colon H^1_\sharp(Y,\mathbf{R}^3)\times M_S \to \mathbf{R}$.

$$J(u, \boldsymbol{E}) := \int_Y W(x, \epsilon(u) + \boldsymbol{E})dx.$$

Let $\boldsymbol{\Sigma}_{ij}$ be the macroscopic stress components:

$$\boldsymbol{\Sigma}_{ij} = \int_Y (2\mu(x)(1 - g(|\boldsymbol{e}|^2))\boldsymbol{e}_{ij} + \left(\lambda(x) + \frac{2\mu(x)}{3} g(|\boldsymbol{e}|^2)\right) \operatorname{tr}(\boldsymbol{e})\delta_{ij})dx$$

where $\boldsymbol{e} = \epsilon(u) + \boldsymbol{E}$.
Problem formulation. Let t be a prescribed macroscopic strain for uniaxial tension direction. The cell problem for the uniaxial tension test is formulated as the equality constrained optimization problem:

$$\begin{cases} \min J(u, \boldsymbol{E}), & \\ \text{subject to} & \boldsymbol{E}_{1,1} = t, \\ & \boldsymbol{\Sigma}_{12} = \boldsymbol{\Sigma}_{13} = \boldsymbol{\Sigma}_{22} = \boldsymbol{\Sigma}_{23} = \boldsymbol{\Sigma}_{33} = 0. \end{cases} \tag{13}$$

where the minimum is taken over the space $H^1_\sharp(Y,\mathbf{R}^3) \times M_S$.

Algorithm. We modify the nonlinear PCG algorithm (Algorithm 1) to solve the cell problem (13) where $\boldsymbol{E}_{11}$ of the macroscopic strain $\boldsymbol{E}$ is given a priori. The solution u and $\boldsymbol{E}_{12}, \ldots, \boldsymbol{E}_{33}$ of (13) satisfies the equality constraints

$$\begin{aligned}
\Sigma_{22} &= 0 = \tau_{22} + \bar{\lambda}t + (2\bar{\mu} + \bar{\lambda})E_{22} + \bar{\lambda}E_{33} \\
\Sigma_{33} &= 0 = \tau_{33} + \bar{\lambda}t + \bar{\lambda}E_{22} + (2\bar{\mu} + \bar{\lambda})E_{33} \\
\Sigma_{12} &= 0 = \tau_{12} + 2\bar{\mu}E_{12} \\
\Sigma_{13} &= 0 = \tau_{13} + 2\bar{\mu}E_{13} \\
\Sigma_{23} &= 0 = \tau_{23} + 2\bar{\mu}E_{23}
\end{aligned}$$

where

$$\tau_{ij} = \int_Y (2\tilde{\mu}(x)\epsilon_{ij} + \tilde{\lambda}(x)\operatorname{tr}(\epsilon)\delta_{ij})dx, \quad \bar{\mu} := \int_Y \tilde{\mu}(x)dx, \quad \bar{\lambda} := \int_Y \tilde{\lambda}(x)dx$$

Thus, we have

$$\begin{aligned}
\begin{bmatrix} E_{22} \\ E_{33} \end{bmatrix} &= -\frac{1}{4\bar{\mu}(\bar{\mu} + \bar{\lambda})} \begin{bmatrix} \bar{\lambda} + 2\bar{\mu} & -\bar{\lambda} \\ -\bar{\lambda} & \bar{\lambda} + 2\bar{\mu} \end{bmatrix} \begin{bmatrix} \tau_{22} + \bar{\lambda}t \\ \tau_{33} + \bar{\lambda}t \end{bmatrix} \\
E_{ij} &= -\frac{\tau_{ij}}{2\bar{\mu}}, \quad i \neq j.
\end{aligned}$$

With this in mind, we modify the PCG algorithm to estimate the macroscopic strain $\boldsymbol{E}$. At k iterate, u^k, $\boldsymbol{E}^k$ being known, we determine $\boldsymbol{E}^{k+1}$ by

$$\begin{cases}
\begin{bmatrix} \boldsymbol{E}_{22}^{k+1} \\ \boldsymbol{E}_{33}^{k+1} \end{bmatrix} = -\dfrac{1}{4\bar{\mu}^k(\bar{\mu}^k + \bar{\lambda}^k)} \begin{bmatrix} \bar{\lambda}^k + 2\bar{\mu}^k & -\bar{\lambda}^k \\ -\bar{\lambda}^k & \bar{\lambda}^k + 2\bar{\mu}^k \end{bmatrix} \begin{bmatrix} \tau_{22}^k + \bar{\lambda}^k t \\ \tau_{33}^k + \bar{\lambda}^k t \end{bmatrix} \\
\boldsymbol{E}_{ij}^{k+1} = -\dfrac{\tau_{ij}^k}{2\bar{\mu}^k}, \quad i \neq j.
\end{cases} \tag{14}$$

Here all quantities with super script k are defined by using u^k and $\boldsymbol{E}^k$.

Algorithm 2: Nonlinear PCG for (13)
Input: Prescribed macroscopic strain $\boldsymbol{E}_{11} = t$
Initialization:
Start with an initial guess u^0 and compute $\boldsymbol{E}_{22}^0, \ldots, \boldsymbol{E}_{23}^0$ by (14)
Compute the steepest ascent g^0 of J at u_0 by (10)
Solve the variational problem (12) for z^0.
Set the initial search direction $d^0 = -z^0$
Main loop:
for $k = 0, 1, 2, \ldots$ **do**
Compute the macroscopic strain $\boldsymbol{E}_{22}^{k+1}, \ldots, \boldsymbol{E}_{23}^{k+1}$ by (14)
Compute the step length $s = \arg\min_{t>0} J(u^k + td^k, \boldsymbol{E}^{k+1})$ and update $u^{k+1} = u^k + sd^k$
Compute the steepest ascent direction $g^{k+1} = (g_1^{k+1}, g_2^{k+1}, g_3^{k+1})$ by (10)
Solve the variational problem (12) for z^{k+1}
Compute the search direction $d^{k+1} = -z^{k+1} + \beta d^k$ for given $\beta > 0$
end for
Output: The macroscopic stress $\boldsymbol{\Sigma}$ by (11)

We confirmed with numerical experiments that the algorithm converges. The details will be reported elsewhere.

Conclusion

We proposed the nonlinear PCG algorithm for solving the cell problem. We also proposed the method to identify the macroscopic strain E for the uniaxial tensile test.

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