Supplementary material for

A novel stabilized NS-FEM formulation for anisotropic double porosity media

Qi Zhang[1], Ze-Yu Wang[1], Zhen-Yu Yin[1], and Yin-Fu Jin[1,2]

[1]Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China
[2]College of Civil and Transportation Engineering, Shenzhen University, Shenzhen, China

This supplementary material is based on the following three references.

1. Semnani, S.J., White, J.A., Borja, R.I., 2016. Thermoplasticity and strain localization in transversely isotropic materials based on anisotropic critical state plasticity. Int. J. Numer. Anal. Meth. Geomech. 40, 2423–2449.

2. Zhao, Y., Semnani, S.J., Yin, Q., Borja, R.I., 2018. On the strength of transversely isotropic rocks. Int. J. Numer. Anal. Meth. Geomech. 42, 1917–1934.

3. Zhang, Q., 2020. Hydromechanical modeling of solid deformation and fluid flow in the transversely isotropic fissured rocks. Computers and Geotechnics 128, 103812.

1 Review of the anisotropic modified Cam-Clay plasticity (AMCC) model for layered material

The elastic tensor $\mathbb{C}^e$ is transversely isotropic due to the existence of the bedding plane, which has the following expression

$$\begin{aligned}\mathbb{C}^e = {} & \lambda^e \mathbf{1}\otimes\mathbf{1} + 2\mu_T \mathbb{I} + a^e\left(\mathbf{1}\otimes\boldsymbol{M} + \boldsymbol{M}\otimes\mathbf{1}\right) \\ & + b^e \boldsymbol{M}\otimes\boldsymbol{M} + 2\left(\mu_L - \mu_T\right)\left(\boldsymbol{M}\odot\mathbf{1} + \mathbf{1}\odot\boldsymbol{M}\right),\end{aligned} \tag{1}$$

where $\mathbf{1}$ is the second-order identity tensor, $\mathbb{I} = \delta_{ik}\delta_{jl}\,\mathbf{e}_i\otimes\mathbf{e}_j\otimes\mathbf{e}_k\otimes\mathbf{e}_l$ is the fourth-order identity tensor, $(\boldsymbol{A}\odot\boldsymbol{B})_{ijkl} = A_{ik}B_{jl}$, $\boldsymbol{M} = \mathbf{n}\otimes\mathbf{n}$, $\mathbf{n}$ is the unit normal vector of the bedding plane, λ^e, μ_L, μ_T, a^e, and b^e are the material elastic constants [1]. The subscript $(\cdot)_T$ means in the isotropic plane and subscript $(\cdot)_L$ means perpendicular to this isotropic plane. It is necessary to mention that when $\mathbf{n} = \mathbf{e}_z = [0,0,1]^T$, the

[1]It could be a little bit strange that why the definitions of $\mathbb{I}$ and $\odot$ are different from the "common" knowledge, *i.e.*, $\mathbb{I}_{ijkl} = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)/2$ and $(\boldsymbol{A}\odot\boldsymbol{B})_{ijkl} = \left(A_{ik}B_{jl} + A_{il}B_{jk}\right)/2$. These "modified" definitions (major symmetry is preserved) are enforced to guarantee the related fourth-order tensors are non-singular by using the notation of Section 3. In addition, as long as we are dealing with symmetric stress and strain tensors, the "modified" definitions would not lead to inconsistencies. There could be alternative ways that will still work without these "modified" definitions, but we will not discuss them here.

Voigt form of $\mathbb{C}^e$ is given by the following 6 by 6 matrix C^e

$$C^e = \begin{bmatrix} \lambda^e + 2\mu_T & \lambda^e & \lambda^e + a^e & & & \\ \lambda^e & \lambda^e + 2\mu_T & \lambda^e + a^e & & & \\ \lambda^e + a^e & \lambda^e + a^e & \lambda^e + 2\tilde{\mu} & & & \\ & & & \mu_T & & \\ & & & & \mu_L & \\ & & & & & \mu_L \end{bmatrix}, \tag{2}$$

where $\tilde{\mu} = 2\mu_L - \mu_T + a^e + b^e/2$. The generalized bulk modulus K^* for the drained transversely isotropic material is given as

$$K^* = \frac{\mathbf{1} : \mathbb{C}^e : \mathbf{1}}{9} = \lambda^e + \frac{2}{9}\mu_T + \frac{4}{9}\mu_L + \frac{2}{3}a^e + \frac{1}{9}b^e \,. \tag{3}$$

The yield function f is given as

$$f(\boldsymbol{\sigma}, p_c) = \frac{\boldsymbol{\sigma} : \mathbb{A} : \boldsymbol{\sigma}}{2M^2} + (\boldsymbol{a} : \boldsymbol{\sigma})(\boldsymbol{a} : \boldsymbol{\sigma} - p_c) \,, \tag{4}$$

where $\mathbb{A} = \mathbb{P} : (3\mathbb{I} - \mathbf{1} \otimes \mathbf{1}) : \mathbb{P}$, and $\mathbb{P} = c_1^p \mathbb{I} + c_2^p \boldsymbol{M} \odot \boldsymbol{M} + c_3^p (\boldsymbol{M} \odot \mathbf{1} + \mathbf{1} \odot \boldsymbol{M})/2$ is the stress projection tensor, c_1^p, c_2^p, and c_3^p are the projection constants, $\boldsymbol{a} = \mathbb{P} : \mathbf{1}/3$, $M = 6\sin\phi_{cs}/(3 - \sin\phi_{cs})$ is the non-zero slope of the critical state line, ϕ_{cs} is the critical state friction angle, $p_c < 0$ is the preconsolidation pressure. Note when $\mathbb{P} = \mathbb{I}$, the yield function would retreat to the standard yield function of MCC. After specifying the yield function f, the plastic strain increment $\mathrm{d}\boldsymbol{\epsilon}^p = \mathrm{d}\boldsymbol{\epsilon} - \mathrm{d}\boldsymbol{\epsilon}^e$ can be calculated using the associative flow rule as

$$\mathrm{d}\boldsymbol{\epsilon}^p = \mathrm{d}\lambda \frac{\partial f}{\partial \boldsymbol{\sigma}} = \mathrm{d}\lambda \left[\frac{\mathbb{A} : \boldsymbol{\sigma}}{M^2} + \boldsymbol{a}(2\boldsymbol{a} : \boldsymbol{\sigma} - p_c) \right], \tag{5}$$

where $\mathrm{d}\lambda \geq 0$ is the plastic scalar multiplier. The last component of this model is the hardening law for p_c, which is given as

$$\mathrm{d}p_c = \frac{p_c}{\lambda^p} \mathrm{d}\epsilon_v^p \,, \tag{6}$$

where $\mathrm{d}\epsilon_v^p = \mathrm{Tr}(\mathrm{d}\boldsymbol{\epsilon}^p)$ and $\lambda^p < 0$ is the plastic compressibility parameter.

2 Return mapping algorithm and algorithmic stress-strain tangent operator

The return mapping algorithm starts by backward Euler integrating plasticity equations (in rate form) from time t_n to t_{n+1}, and a group of coupled equations with unknowns $\boldsymbol{\sigma}$, $\Delta\lambda$, and p_c could be obtained

$$-\left(\boldsymbol{\sigma}^{\mathrm{old}} + \mathbb{C}^e : \Delta\boldsymbol{\epsilon}\right) + \mathbb{C}^e : \left(\Delta\lambda \frac{\partial f}{\partial \boldsymbol{\sigma}}\right) + \boldsymbol{\sigma} = \mathbf{0} \,, \tag{7}$$

$$p_c^{\mathrm{old}} \exp\left[\frac{\Delta\lambda\, \mathrm{Tr}(\partial f/\partial\boldsymbol{\sigma})}{\lambda^p}\right] - p_c = 0 \,, \tag{8}$$

$$f(\boldsymbol{\sigma}, p_c) = 0 \,, \tag{9}$$

where the superscript marks old physical variables, and all the other physical variables are at time t_{n+1}.

The second step of the return mapping algorithm is to check whether plastic deformation could accumulate. First of all, trial solutions are constructed as $\boldsymbol{\sigma}^{\mathrm{trial}} = \boldsymbol{\sigma}^{\mathrm{old}} + \mathbb{C}^e : \Delta\boldsymbol{\epsilon}$ and $p_c^{\mathrm{trial}} = p_c^{\mathrm{old}}$. Next, the

trial solutions are substituted into the yield function f. Finally, if $f \leq 0$, then we are in the elastic range and we don't need to solve above coupled equations, the $\mathbb{C}^{\text{algo}}$ is equal to the $\mathbb{C}^e$, otherwise, we proceed to the third step.

In the third step, pure Newton's method is applied to solve above coupled equations simultaneously provided $f > 0$. To illustrate this method more efficiently, full matrix/vector notation is adopted, see Section 3. Following this notation, $x \in \mathbb{R}^9$, $y \in \mathbb{R}$, and $z \in \mathbb{R}$ are used to represent $\boldsymbol{\sigma}$, $\Delta\lambda$, and p_c, respectively. Also, the original $\mathbb{C}^e$ is transformed to symmetric $C^e \in \mathbb{R}^{9\times 9}$, the fourth-order identity tensor $\mathbb{I}$ is transformed to identity matrix $I \in \mathbb{R}^{9\times 9}$, the second-order identity tensor $\mathbf{1}$ is transformed to $I_2 \in \mathbb{R}^9$, $\boldsymbol{\sigma}^{\text{trial}}$ is transformed to $\sigma^{\text{trial}} \in \mathbb{R}^9$, $\mathbb{A}$ is transformed to symmetric $A \in \mathbb{R}^{9\times 9}$, and $\boldsymbol{a}$ is transformed to $a \in \mathbb{R}^9$. In Newton's method, the residual vector $g \in \mathbb{R}^{11}$ and Hessian matrix $J \in \mathbb{R}^{11\times 11}$ are constructed for every iteration. Suppose the superscript v with parentheses is used to represent iteration counter where $v = 0$ means the initial guess, then for each v, we need to solve following block linear equations to obtain the Newton's step $\left[\delta x^T, \delta y, \delta z\right]^T$ and update $\left[x^{(v+1)^T}, y^{(v+1)}, z^{(v+1)}\right]^T = \left[x^{(v)^T}, y^{(v)}, z^{(v)}\right]^T + \left[\delta x^T, \delta y, \delta z\right]^T$ for next iteration

$$\begin{bmatrix} J_{11}^{(v)} & J_{12}^{(v)} & J_{13}^{(v)} \\ J_{21}^{(v)} & J_{22}^{(v)} & J_{23}^{(v)} \\ J_{31}^{(v)} & J_{32}^{(v)} & J_{33}^{(v)} \end{bmatrix} \begin{bmatrix} \delta x \\ \delta y \\ \delta z \end{bmatrix} = \begin{bmatrix} -g_1^{(v)} \\ -g_2^{(v)} \\ -g_3^{(v)} \end{bmatrix}, \tag{10}$$

where $g_1^{(v)} \in \mathbb{R}^9$, $g_2^{(v)} \in \mathbb{R}$, and $g_3^{(v)} \in \mathbb{R}$ are block vectors of the residual vector g, $J_{11}^{(v)} \in \mathbb{R}^{9\times 9}$, $J_{12}^{(v)} \in \mathbb{R}^{9\times 1}$, $J_{13}^{(v)} \in \mathbb{R}^{9\times 1}$, $J_{21}^{(v)} \in \mathbb{R}^{1\times 9}$, $J_{22}^{(v)} \in \mathbb{R}$, $J_{23}^{(v)} \in \mathbb{R}$, $J_{31}^{(v)} \in \mathbb{R}^{1\times 9}$, $J_{32}^{(v)} \in \mathbb{R}$, and $J_{33}^{(v)} \in \mathbb{R}$ are block matrices of the Hessian matrix J. The expressions for these block elements are given in Section 4.

In the last step of the return mapping algorithm, when the stopping criterion is satisfied, we are ready to use the updated $\boldsymbol{\sigma}$, $\Delta\lambda$, and p_c (same as $x^{(\text{last})}$, $y^{(\text{last})}$, and $z^{(\text{last})}$) to calculate $\mathbb{C}^{\text{algo}}$ in the 9×9 matrix form C^{algo}. The procedure is given here. First of all, $x_1 \in \mathbb{R}^9$ and $x_2 \in \mathbb{R}^9$ are solved such that they satisfy following linear equations (18×18)

$$\begin{bmatrix} \left(J_{21}J_{11}^{-1}J_{12} - J_{22}\right) I & \left(J_{21}J_{11}^{-1}J_{13} - J_{23}\right) I \\ \left(J_{31}J_{11}^{-1}J_{12}\right) I & \left(J_{31}J_{11}^{-1}J_{13} - J_{33}\right) I \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \left(J_{21}J_{11}^{-1}C^e\right)^T \\ \left(J_{31}J_{11}^{-1}C^e\right)^T \end{bmatrix}. \tag{11}$$

As mentioned before, J is evaluated at the termination of the Newton's method. After obtaining x_1 and x_2, C^{algo} can be calculated easily as

$$C^{\text{algo}} = J_{11}^{-1}C^e - J_{11}^{-1}J_{12}x_1^T - J_{11}^{-1}J_{13}x_2^T. \tag{12}$$

It is also necessary to mention that although the analytical formula for $\mathbb{C}^{\text{algo}}$ is derived, it is given in the full 9×9 matrix form (C^{algo}), thus a transformation to the traditional 6×6 matrix form is necessary, please see Section 3 for more details.

As a final note of this section, in Section 5, the complete calculation results of a typical uniaxial strain point simulation in 3D after 5 incremental loading steps with the same $\Delta\boldsymbol{\epsilon}$ is provided. Any other return mapping algorithms should be able to reproduce exactly the same results before they are used in real problems.

3 Full matrix/vector notation

In this notation, the second-order tensors such as stress and strain are stored in column vectors such as $x \in \mathbb{R}^9$, and the fourth-order tensors are stored in matrices such as $C \in \mathbb{R}^{9\times 9}$, thus the transformation

rule needs to be stated, *i.e.*, the correspondence $\alpha \leftrightarrow ij$ and $\beta \leftrightarrow kl$ where $\alpha, \beta = 1, 2, \ldots, 9$ and $i, j, k, l = 1, 2, 3$, see following Table 1. Given a 9×9 stiffness matrix C, the aim is to output the equivalent 6×6

Table 1: Transformation rule.

Vector indices α and β	1	2	3	4	5	6	7	8	9
Tensor index pairs ij and kl	11	21	31	12	22	32	13	23	33

stiffness matrix $\hat{C}$. To accomplish that, a matrix $E \in \mathbb{R}^{9\times 6}$ is defined as follows

$$E = \begin{bmatrix} e_1 & e_5 & e_9 & (e_2 + e_4)/2 & (e_3 + e_7)/2 & (e_6 + e_8)/2 \end{bmatrix}, \tag{13}$$

where $e_i \in \mathbb{R}^9$ for $i = 1, 2, \ldots, 9$ are unit vectors in the 9 dimensional space, and e_i means that only the i^{th} component is 1, all the other components are 0. Next we do the matrix multiplication and obtain $B = CE$ that is also a 9×6 matrix. Let us rewrite B using row representations $b_j \in \mathbb{R}^6$ for $j = 1, 2, \ldots, 9$, now $\hat{C}$ is represented as

$$\hat{C} = \begin{pmatrix} b_1^T \\ b_5^T \\ b_9^T \\ b_4^T/2 + b_2^T/2 \\ b_7^T/2 + b_3^T/2 \\ b_8^T/2 + b_6^T/2 \end{pmatrix}, \tag{14}$$

which is a 6×6 matrix. Here the default order of the Voigt notation is 11, 22, 33, 12, 13, 23. In Cartesian coordinate system, the order is described as xx, yy, zz, xy, xz, yz. It is also important to mention that above procedure only applies to the stiffness matrix. For compliance matrix, please drop the "/2" in Eq. (13), and multiply the last three rows of $\hat{C}$ in Eq. (14) by 2.

4 Residual vector and Hessian matrix for the return mapping algorithm

The following expressions are used in the Eq. (10)

$$g_1^{(v)} = x^{(v)} + y^{(v)} C^e \left[\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right) \right] - \sigma^{\text{trial}}, \tag{15}$$

$$g_2^{(v)} = p_c^{\text{old}} \exp\left[\frac{y^{(v)}}{\lambda^p} I_2^T \left(\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right) \right) \right] - z^{(v)}, \tag{16}$$

$$g_3^{(v)} = \frac{{x^{(v)}}^T A x^{(v)}}{2M^2} + a^T x^{(v)} \left(a^T x^{(v)} - z^{(v)}\right), \tag{17}$$

$$J_{11}^{(v)} = I + y^{(v)} C^e \left(\frac{A}{M^2} + 2aa^T \right), \tag{18}$$

$$J_{12}^{(v)} = C^e \left[\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right) \right], \tag{19}$$

$$J_{13}^{(v)} = -y^{(v)} C^e a, \tag{20}$$

$$J_{21}^{(v)} = \frac{y^{(v)} p_c^{\text{old}}}{\lambda^p} \exp\left[\frac{y^{(v)}}{\lambda^p} I_2^T \left(\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right)\right)\right] I_2^T \left(\frac{A}{M^2} + 2aa^T\right), \tag{21}$$

$$J_{22}^{(v)} = \frac{p_c^{\text{old}}}{\lambda^p} \exp\left[\frac{y^{(v)}}{\lambda^p} I_2^T \left(\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right)\right)\right] I_2^T \left[\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right)\right], \tag{22}$$

$$J_{23}^{(v)} = -\frac{y^{(v)} p_c^{\text{old}}}{\lambda^p} \exp\left[\frac{y^{(v)}}{\lambda^p} I_2^T \left(\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right)\right)\right] I_2^T a - 1, \tag{23}$$

$$J_{31}^{(v)} = \left[\frac{Ax^{(v)}}{M^2} + a\left(2a^T x^{(v)} - z^{(v)}\right)\right]^T, \tag{24}$$

$$J_{32}^{(v)} = 0, \tag{25}$$

$$J_{33}^{(v)} = -a^T x^{(v)}. \tag{26}$$

5 Benchmark strain point simulation

In this strain point simulation, we assume $\boldsymbol{a} = \mathbb{P} : \mathbf{1}/3$ and following material parameters that are similar to those of Tournemire shale: $\lambda^e = 4270$ MPa, $\mu_T = 9360$ MPa, $\mu_L = 6510$ MPa, $a^e = -1870$ MPa, $b^e = 5420$ MPa, $M = 1.07$, $\lambda^p = -0.0026$, $c_1^p = 0.7$, $c_2^p = -0.36$, and $c_3^p = 0.6$. The bedding plane angle is $\pi/3$ in $x\mathrm{O}y$ plane, which leads to $\mathbf{n} = \left[-\sqrt{3}/2, 1/2, 0\right]^T$ and following elastic stiffness matrix $\hat{C}^e \in \mathbb{R}^{6\times 6}$ (the default unit is MPa)

$$\hat{C}^e = \begin{bmatrix} 14683.75 & 3416.25 & 2867.50 & 1517.71 & 0 & 0 \\ 3416.25 & 19543.75 & 3802.50 & 2691.17 & 0 & 0 \\ 2867.50 & 3802.50 & 22990.00 & 809.73 & 0 & 0 \\ 1517.71 & 2691.17 & 809.73 & 7526.25 & 0 & 0 \\ 0 & 0 & 0 & 0 & 7222.50 & 1234.09 \\ 0 & 0 & 0 & 0 & 1234.09 & 8647.50 \end{bmatrix}. \tag{27}$$

For the stress history, the initial p_c is -40 MPa. The loading procedures are described as follows. First of all, the material is subject to an isotropic compression of -10 MPa, which leads to a non-zero initial strain, *i.e.*, $\boldsymbol{\epsilon}_0 \neq \mathbf{0}$. Next, we prescribe the same strain increment $\Delta\boldsymbol{\epsilon}$ at each step, and repeat it for 5 times. The $\Delta\boldsymbol{\epsilon}$ is given as

$$\Delta\boldsymbol{\epsilon} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -0.001 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{28}$$

That is to say, only axial deformation in the y-direction is allowed. As a result, only the first step is an elastic step and the other four steps are plastic steps. For benchmark verification, the final values of p_c, $\boldsymbol{\epsilon}$, $\boldsymbol{\sigma}$, and $\hat{C}^{\text{algo}} \in \mathbb{R}^{6\times 6}$ after 5 steps are provided here (the default unit is MPa except for $\boldsymbol{\epsilon}$)

$$p_c = -50.7379, \tag{29}$$

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}_0 + 5\Delta\boldsymbol{\epsilon} = 10^{-3} \times \begin{bmatrix} -0.55858 & 0.14330 & 0 \\ 0.14330 & -5.39311 & 0 \\ 0 & 0 & -0.31038 \end{bmatrix}, \tag{30}$$

$$\boldsymbol{\sigma} = \begin{bmatrix} -35.87171 & -10.03319 & 0 \\ -10.03319 & -68.64135 & 0 \\ 0 & 0 & -39.60607 \end{bmatrix}, \tag{31}$$

$$\hat{\boldsymbol{C}}^{\text{algo}} = \begin{bmatrix} 10992.87 & 4912.10 & 3186.54 & 1191.42 & 0 & 0 \\ 6238.00 & 7999.32 & 6613.18 & 883.05 & 0 & 0 \\ 3134.83 & 5692.87 & 17526.77 & 895.95 & 0 & 0 \\ 1384.35 & 1290.07 & 1013.99 & 4991.39 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4786.39 & 1097.03 \\ 0 & 0 & 0 & 0 & 1097.03 & 6053.13 \end{bmatrix}. \tag{32}$$

Here $\hat{\boldsymbol{C}}^{\text{algo}}$ is not symmetric albeit the flow rule is associative. This is because of the form of the incremental hardening law Eq. (8). In addition, here the order of the Voigt notation is xx, yy, zz, xy, xz, yz.

6 Coordinate transformation of the stiffness matrix

For a vertically transversely isotropic (VTI) material whose plane of isotropy is the $x\mathrm{O}y$ plane, the stress-strain relation is given as:

$$\begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \sigma_{xy} \\ \sigma_{xz} \\ \sigma_{yz} \end{Bmatrix}_{\text{local,TTI}} = \begin{bmatrix} \frac{1}{E_h} & -\frac{\nu_{hh}}{E_h} & -\frac{\nu_{vh}}{E_v} & & & \\ -\frac{\nu_{hh}}{E_h} & \frac{1}{E_h} & -\frac{\nu_{vh}}{E_v} & & & \\ -\frac{\nu_{hv}}{E_h} & -\frac{\nu_{hv}}{E_h} & \frac{1}{E_v} & & & \\ & & & \frac{2(1+\nu_{hh})}{E_h} & & \\ & & & & \frac{1}{G_{vh}} & \\ & & & & & \frac{1}{G_{vh}} \end{bmatrix}^{-1}_{\text{local,TTI}} \begin{Bmatrix} \epsilon_x \\ \epsilon_y \\ \epsilon_z \\ 2\epsilon_{xy} \\ 2\epsilon_{xz} \\ 2\epsilon_{yz} \end{Bmatrix}_{\text{local,TTI}}, \tag{33}$$

Note that the above representation depends on the ordering of shear, here in assumed as "xy, xz, yz". Now for a tilted transversely isotropic (TTI) material, Eq. (33) only holds in the local coordinate system. The basis vectors of this local coordinate system are assumed to be $\{\boldsymbol{e}_1', \boldsymbol{e}_2', \boldsymbol{e}_3'\}$. By convention, "1" means x in local system or global system, "2" means y, and "3" means z. Of course, we know the normal vector of the isotropy plane is $\boldsymbol{e}_3'$. The global coordinate system has basis vectors $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$. The stiffness matrix in Eq. (33) will be denoted as $\boldsymbol{M}'$. The relation between two groups of basis vectors is given by an orthogonal matrix $\boldsymbol{Q}$:

$$\boldsymbol{e}_1' = Q_{11}\boldsymbol{e}_1 + Q_{21}\boldsymbol{e}_2 + Q_{31}\boldsymbol{e}_3, \tag{34}$$

$$\boldsymbol{e}_2' = Q_{12}\boldsymbol{e}_1 + Q_{22}\boldsymbol{e}_2 + Q_{32}\boldsymbol{e}_3, \tag{35}$$

$$\boldsymbol{e}_3' = Q_{13}\boldsymbol{e}_1 + Q_{23}\boldsymbol{e}_2 + Q_{33}\boldsymbol{e}_3, \tag{36}$$

where Q_{ij} is exactly the element of row i and column j of $\boldsymbol{Q}$:

$$\boldsymbol{Q} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix}. \tag{37}$$

The previous three equations can also be written as (note that the bold-faced $\boldsymbol{e}$ is NOT a scalar!)

$$\begin{bmatrix} \boldsymbol{e}_1' & \boldsymbol{e}_2' & \boldsymbol{e}_3' \end{bmatrix} = \begin{bmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \end{bmatrix} \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix}. \tag{38}$$

Briefly speaking, the i^{th} column of $\boldsymbol{Q}$ is just the representation of $\boldsymbol{e}_i'$ in $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ coordinate system. Now we are ready to get the stiffness matrix $\boldsymbol{M}$ in the global coordinate system. First of all, we rewrite all the elements of $\boldsymbol{Q}$ in terms of ℓ_1 to n_3:

$$\boldsymbol{Q}^T = \begin{bmatrix} Q_{11} & Q_{21} & Q_{31} \\ Q_{12} & Q_{22} & Q_{32} \\ Q_{13} & Q_{23} & Q_{33} \end{bmatrix} = \begin{bmatrix} \ell_1 & m_1 & n_1 \\ \ell_2 & m_2 & n_2 \\ \ell_3 & m_3 & n_3 \end{bmatrix}. \tag{39}$$

Then we define the matrix $\boldsymbol{R}$ as:

$$\boldsymbol{R} = \begin{bmatrix} \ell_1^2 & m_1^2 & n_1^2 & \ell_1 m_1 & n_1 \ell_1 & m_1 n_1 \\ \ell_2^2 & m_2^2 & n_2^2 & \ell_2 m_2 & n_2 \ell_2 & m_2 n_2 \\ \ell_3^2 & m_3^2 & n_3^2 & \ell_3 m_3 & n_3 \ell_3 & m_3 n_3 \\ 2\ell_1\ell_2 & 2m_1 m_2 & 2n_1 n_2 & \ell_1 m_2 + \ell_2 m_1 & n_1 \ell_2 + n_2 \ell_1 & m_1 n_2 + m_2 n_1 \\ 2\ell_3\ell_1 & 2m_3 m_1 & 2n_3 n_1 & \ell_3 m_1 + \ell_1 m_3 & n_3 \ell_1 + n_1 \ell_3 & m_3 n_1 + m_1 n_3 \\ 2\ell_2\ell_3 & 2m_2 m_3 & 2n_2 n_3 & \ell_2 m_3 + \ell_3 m_2 & n_2 \ell_3 + n_3 \ell_2 & m_2 n_3 + m_3 n_2 \end{bmatrix}. \tag{40}$$

So:

$$\boldsymbol{M} = \boldsymbol{R}^T \boldsymbol{M}' \boldsymbol{R}. \tag{41}$$

Again, this matrix $\boldsymbol{R}$ is a little bit different from that in Xu et al. (2021), and this is also due to the ordering of shear, here we assume "xy, xz, yz". There is one more interesting property of $\boldsymbol{R}$, which is (see off-diagonal 3×3 blocks):

$$\boldsymbol{R}^{-T} = \begin{bmatrix} \ell_1^2 & m_1^2 & n_1^2 & 2\ell_1 m_1 & 2n_1 \ell_1 & 2m_1 n_1 \\ \ell_2^2 & m_2^2 & n_2^2 & 2\ell_2 m_2 & 2n_2 \ell_2 & 2m_2 n_2 \\ \ell_3^2 & m_3^2 & n_3^2 & 2\ell_3 m_3 & 2n_3 \ell_3 & 2m_3 n_3 \\ \ell_1\ell_2 & m_1 m_2 & n_1 n_2 & \ell_1 m_2 + \ell_2 m_1 & n_1 \ell_2 + n_2 \ell_1 & m_1 n_2 + m_2 n_1 \\ \ell_3\ell_1 & m_3 m_1 & n_3 n_1 & \ell_3 m_1 + \ell_1 m_3 & n_3 \ell_1 + n_1 \ell_3 & m_3 n_1 + m_1 n_3 \\ \ell_2\ell_3 & m_2 m_3 & n_2 n_3 & \ell_2 m_3 + \ell_3 m_2 & n_2 \ell_3 + n_3 \ell_2 & m_2 n_3 + m_3 n_2 \end{bmatrix}. \tag{42}$$

Finally, as an aside, we recall the vectorial transformation law and tensorial transformation law ($\tilde{\circ}$ implies along the directions $\{\boldsymbol{e}_1', \boldsymbol{e}_2', \boldsymbol{e}_3'\}$):

$$[\tilde{\mathbf{u}}] = [\boldsymbol{Q}]^T [\mathbf{u}], \tag{43}$$

$$[\mathbf{u}] = [\boldsymbol{Q}][\tilde{\mathbf{u}}], \tag{44}$$

$$[\tilde{\boldsymbol{A}}] = [\boldsymbol{Q}]^T [\boldsymbol{A}][\boldsymbol{Q}], \tag{45}$$

$$[\boldsymbol{A}] = [\boldsymbol{Q}][\tilde{\boldsymbol{A}}][\boldsymbol{Q}]^T, \tag{46}$$

$$\tilde{A}_{i_1 i_2 \ldots i_n} = Q_{j_1 i_1} Q_{j_2 i_2} \ldots Q_{j_n i_n} A_{j_1 j_2 \ldots j_n}. \tag{47}$$

7 Simulation code availability statement

We have made our code publicly available from this GitHub page under the **Releases** menu. Please remember to cite the corresponding paper if you use any of these codes for research or industrial purposes.