Appendix A
Matrix Forms of Tensors

A.1 Vector Form for Second-Order Tensors

Let $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ be two symmetric second-order tensors:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix}. \tag{A.1}$$

The vector form $[\boldsymbol{\sigma}]$ associated to $\boldsymbol{\sigma}$ and $[\boldsymbol{\varepsilon}]$ associated to $\boldsymbol{\varepsilon}$ are constructed such that they contain only the independent components of the related tensors as values and such that

$$\boldsymbol{\sigma} : \boldsymbol{\varepsilon} = [\boldsymbol{\sigma}] \cdot [\boldsymbol{\varepsilon}] \tag{A.2}$$

is verified. In 3D, we obtain a first form, called Voigt's notation, and which is used in most of available FEM codes:

$$[\boldsymbol{\sigma}] = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{13} \\ \sigma_{23} \\ \sigma_{12} \end{bmatrix} \text{ and } [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{13} \\ 2\varepsilon_{23} \\ 2\varepsilon_{12} \end{bmatrix}. \tag{A.3}$$

The advantage of such form is that no multiplicative coefficients need to be introduced in the matrix of shape function derivatives (see Chapter 2, (2.99)) to relate the

J. Yvonnet, *Computational Homogenization of Heterogeneous Materials with Finite Elements*, Solid Mechanics and Its Applications 258,
https://doi.org/10.1007/978-3-030-18383-7

strain vector to nodal displacements. Another notation (sometimes called modified Voigt's notation in the literature) is preferred by some authors as it preserves the symmetry of the vector forms as

$$[\boldsymbol{\sigma}] = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sqrt{2}\sigma_{13} \\ \sqrt{2}\sigma_{23} \\ \sqrt{2}\sigma_{12} \end{bmatrix} \text{ and } [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\varepsilon_{13} \\ \sqrt{2}\varepsilon_{23} \\ \sqrt{2}\varepsilon_{12} \end{bmatrix}. \tag{A.4}$$

In 2D, the stress and strain tensors reduce to

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{12} & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}, \quad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ \varepsilon_{12} & \varepsilon_{22} & 0 \\ 0 & 0 & \varepsilon_{33} \end{bmatrix}. \tag{A.5}$$

If plane strain ($\varepsilon_{33} = 0$) or plane stress ($\sigma_{33} = 0$) assumption is considered, then the product $\varepsilon_{33}\sigma_{33}$ vanishes in both cases. It is, thus, not necessary to include ε_{33} and σ_{33} in the analysis, as then can be deduced from the other components. Then, the vector forms are simply provided by

$$[\boldsymbol{\sigma}] = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} \text{ and } [\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{bmatrix} \text{ (Voigt's notation)}, \tag{A.6}$$

or

$$[\boldsymbol{\varepsilon}] = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \sqrt{2}\varepsilon_{12} \end{bmatrix} \text{ (Modified Voigt's notation)}. \tag{A.7}$$

A.2 Matrix Form for Fourth-Order Tensors

The matrix form of fourth-order tensor relates the vector forms of second-order tensors. For example, expressing the Hooke's law,

$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}, \quad \text{or } \sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \tag{A.8}$$

and considering the symmetries of $\boldsymbol{\varepsilon}$ and $\mathbb{C}$, it gives, in 3D:

$$\sigma_{11} = C_{1111}\varepsilon_{11} + C_{1122}\varepsilon_{22} + C_{1133}\varepsilon_{33} + 2C_{1113}\varepsilon_{13} + 2C_{1123}\varepsilon_{23} + 2C_{1112}\varepsilon_{12} \tag{A.9}$$

$$\sigma_{22} = C_{1122}\varepsilon_{11} + C_{2222}\varepsilon_{22} + C_{2233}\varepsilon_{33} + 2C_{2213}\varepsilon_{13} + 2C_{2223}\varepsilon_{23} + 2C_{2212}\varepsilon_{12} \tag{A.10}$$

$$\sigma_{33} = C_{1133}\varepsilon_{11} + C_{2233}\varepsilon_{22} + C_{3333}\varepsilon_{33} + 2C_{3313}\varepsilon_{13} + 2C_{3323}\varepsilon_{23} + 2C_{3312}\varepsilon_{12} \tag{A.11}$$

$$\sigma_{13} = C_{1113}\varepsilon_{11} + C_{2213}\varepsilon_{22} + C_{3313}\varepsilon_{33} + 2C_{1313}\varepsilon_{13} + 2C_{1323}\varepsilon_{23} + 2C_{1312}\varepsilon_{12} \tag{A.12}$$

$$\sigma_{23} = C_{1123}\varepsilon_{11} + C_{2223}\varepsilon_{22} + C_{3323}\varepsilon_{33} + 2C_{1323}\varepsilon_{13} + 2C_{2323}\varepsilon_{23} + 2C_{2312}\varepsilon_{12} \tag{A.13}$$

$$\sigma_{12} = C_{1112}\varepsilon_{11} + C_{2212}\varepsilon_{22} + C_{3312}\varepsilon_{33} + 2C_{1312}\varepsilon_{13} + 2C_{2312}\varepsilon_{23} + 2C_{1212}\varepsilon_{12}. \tag{A.14}$$

Then, using (A.3) (Voigt's notation), we obtain

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{13} \\ \sigma_{23} \\ \sigma_{12} \end{bmatrix} = \underbrace{\begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1113} & C_{1123} & C_{1112} \\ C_{1122} & C_{2222} & C_{2233} & C_{2213} & C_{2223} & C_{2212} \\ C_{1133} & C_{2233} & C_{3333} & C_{3313} & C_{3323} & C_{3312} \\ C_{1113} & C_{2213} & C_{3313} & C_{1313} & C_{1323} & C_{1312} \\ C_{1123} & C_{2223} & C_{3323} & C_{1323} & C_{2323} & C_{2312} \\ C_{1112} & C_{2212} & C_{3312} & C_{1312} & C_{2312} & C_{1212} \end{bmatrix}}_{\mathbf{C}} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{13} \\ 2\varepsilon_{23} \\ 2\varepsilon_{12} \end{bmatrix}, \tag{A.15}$$

where $\mathbf{C}$ is the matrix form associated with the fourth-order elastic tensor $\mathbb{C}$. Using the alternative form (A.4) (modified Voigt's notation), we obtain

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sqrt{2}\sigma_{13} \\ \sqrt{2}\sigma_{23} \\ \sqrt{2}\sigma_{12} \end{bmatrix} = \underbrace{\begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1113} & \sqrt{2}C_{1123} & \sqrt{2}C_{1112} \\ C_{1122} & C_{2222} & C_{2233} & \sqrt{2}C_{2213} & \sqrt{2}C_{2223} & \sqrt{2}C_{2212} \\ C_{1133} & C_{2233} & C_{3333} & \sqrt{2}C_{3313} & \sqrt{2}C_{3323} & \sqrt{2}C_{3312} \\ \sqrt{2}C_{1113} & \sqrt{2}C_{2213} & \sqrt{2}C_{3313} & 2C_{1313} & 2C_{1323} & 2C_{1312} \\ \sqrt{2}C_{1123} & \sqrt{2}C_{2223} & \sqrt{2}C_{3323} & 2C_{1323} & 2C_{2323} & 2C_{2312} \\ \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & \sqrt{2}C_{3312} & 2C_{1312} & 2C_{2312} & 2C_{1212} \end{bmatrix}}_{\mathbf{C}} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\varepsilon_{13} \\ \sqrt{2}\varepsilon_{23} \\ \sqrt{2}\varepsilon_{12} \end{bmatrix}. \tag{A.16}$$

In 2D, it gives

$$\sigma_{11} = C_{1111}\varepsilon_{11} + C_{1122}\varepsilon_{22} + C_{1133}\varepsilon_{33} + 2C_{1112}\varepsilon_{12} \tag{A.17}$$

$$\sigma_{22} = C_{1122}\varepsilon_{11} + C_{2222}\varepsilon_{22} + C_{2233}\varepsilon_{33} + 2C_{2212}\varepsilon_{12} \tag{A.18}$$

$$\sigma_{33} = C_{1133}\varepsilon_{11} + C_{2233}\varepsilon_{22} + C_{3333}\varepsilon_{33} + 2C_{3312}\varepsilon_{12} \tag{A.19}$$

$$\sigma_{12} = C_{1112}\varepsilon_{11} + C_{2212}\varepsilon_{22} + C_{3312}\varepsilon_{33} + 2C_{1212}\varepsilon_{12}. \tag{A.20}$$

The corresponding matrix form is then given for the Voigt's notation by

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ \sigma_{33} \end{bmatrix} = \underbrace{\begin{bmatrix} C_{1111} & C_{1122} & C_{1112} & C_{1133} \\ C_{1122} & C_{2222} & C_{2212} & C_{2233} \\ C_{1112} & C_{2212} & C_{1212} & C_{3312} \\ C_{1133} & C_{2233} & C_{3312} & C_{3333} \end{bmatrix}}_{\mathbf{C}} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \\ \varepsilon_{33} \end{bmatrix}. \tag{A.21}$$

Considering plane strains:

$$\sigma_{11} = C_{1111}\varepsilon_{11} + C_{1122}\varepsilon_{22} + 2C_{1112}\varepsilon_{12} \tag{A.22}$$

$$\sigma_{22} = C_{1122}\varepsilon_{11} + C_{2222}\varepsilon_{22} + 2C_{2212}\varepsilon_{12} \tag{A.23}$$

$$\sigma_{12} = C_{1112}\varepsilon_{11} + C_{2212}\varepsilon_{22} + 2C_{1212}\varepsilon_{12}, \tag{A.24}$$

and the corresponding matrix form is then given for the Voigt's notation by

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} = \underbrace{\begin{bmatrix} C_{1111} & C_{1122} & C_{1112} \\ C_{1122} & C_{2222} & C_{2212} \\ C_{1112} & C_{2212} & C_{1212} \end{bmatrix}}_{\mathbf{C}} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{bmatrix}, \tag{A.25}$$

and in modified Voigt's notation by

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sqrt{2}\sigma_{12} \end{bmatrix} = \underbrace{\begin{bmatrix} C_{1111} & C_{1122} & \sqrt{2}C_{1112} \\ C_{1122} & C_{2222} & \sqrt{2}C_{2212} \\ \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & 2C_{1212} \end{bmatrix}}_{\mathbf{C}} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \sqrt{2}\varepsilon_{12} \end{bmatrix}. \tag{A.26}$$

A.3 Matrix Forms for Third-Order Tensors

An example of third-order tensor can be found in piezoelectricity (see Chap. 5). Considering, Eq. (5.7) without external electric field, we have the relationship:

$$D_i = \mathscr{E}_{ijk}\varepsilon_{jk}. \tag{A.27}$$

Expanding the above equation:

$$D_1 = \mathscr{E}_{111}\varepsilon_{11} + \mathscr{E}_{122}\varepsilon_{22} + \mathscr{E}_{133}\varepsilon_{33} + 2\mathscr{E}_{113}\varepsilon_{13} + 2\mathscr{E}_{123}\varepsilon_{23} + 2\mathscr{E}_{112}\varepsilon_{12} \tag{A.28}$$

$$D_2 = \mathscr{E}_{211}\varepsilon_{11} + \mathscr{E}_{222}\varepsilon_{22} + \mathscr{E}_{233}\varepsilon_{33} + 2\mathscr{E}_{213}\varepsilon_{13} + 2\mathscr{E}_{223}\varepsilon_{23} + 2\mathscr{E}_{212}\varepsilon_{12} \tag{A.29}$$

$$D_3 = \mathscr{E}_{311}\varepsilon_{11} + \mathscr{E}_{322}\varepsilon_{22} + \mathscr{E}_{333}\varepsilon_{33} + 2\mathscr{E}_{313}\varepsilon_{13} + 2\mathscr{E}_{323}\varepsilon_{23} + 2\mathscr{E}_{312}\varepsilon_{12}, \tag{A.30}$$

we can express the matrix form $[\mathscr{E}]$ associated with $\mathscr{E}$, using the Voigt's notation, as

$$\begin{bmatrix} D_1 \\ D_2 \\ D_3 \end{bmatrix} = \underbrace{\begin{bmatrix} \mathscr{E}_{111} & \mathscr{E}_{122} & \mathscr{E}_{133} & \mathscr{E}_{113} & \mathscr{E}_{123} & \mathscr{E}_{112} \\ \mathscr{E}_{211} & \mathscr{E}_{222} & \mathscr{E}_{233} & \mathscr{E}_{213} & \mathscr{E}_{223} & \mathscr{E}_{212} \\ \mathscr{E}_{311} & \mathscr{E}_{322} & \mathscr{E}_{333} & \mathscr{E}_{313} & \mathscr{E}_{323} & \mathscr{E}_{312} \end{bmatrix}}_{[\mathscr{E}]} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{13} \\ 2\varepsilon_{23} \\ 2\varepsilon_{12} \end{bmatrix}. \tag{A.31}$$

In 2D we have, considering out-of-plane effects:

$$\begin{bmatrix} D_1 \\ D_2 \\ D_3 \end{bmatrix} = \underbrace{\begin{bmatrix} \mathscr{E}_{111} & \mathscr{E}_{122} & \mathscr{E}_{133} & \mathscr{E}_{112} \\ \mathscr{E}_{211} & \mathscr{E}_{222} & \mathscr{E}_{233} & \mathscr{E}_{212} \\ \mathscr{E}_{311} & \mathscr{E}_{322} & \mathscr{E}_{333} & \mathscr{E}_{312} \end{bmatrix}}_{[\mathscr{E}]} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{12} \end{bmatrix}, \tag{A.32}$$

and for 2D plane strains (Voigt's notation)

$$\begin{bmatrix} D_1 \\ D_2 \end{bmatrix} = \underbrace{\begin{bmatrix} \mathscr{E}_{111} & \mathscr{E}_{122} & \mathscr{E}_{112} \\ \mathscr{E}_{211} & \mathscr{E}_{222} & \mathscr{E}_{212} \end{bmatrix}}_{[\mathscr{E}]} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \end{bmatrix}. \tag{A.33}$$

Using the modified Voigt's notation (A.4), we obtain

$$\begin{bmatrix} D_1 \\ D_2 \\ D_3 \end{bmatrix} = \underbrace{\begin{bmatrix} \mathscr{E}_{111} & \mathscr{E}_{122} & \mathscr{E}_{133} & \sqrt{2}\mathscr{E}_{113} & \sqrt{2}\mathscr{E}_{123} & \sqrt{2}\mathscr{E}_{112} \\ \mathscr{E}_{211} & \mathscr{E}_{222} & \mathscr{E}_{233} & \sqrt{2}\mathscr{E}_{213} & \sqrt{2}\mathscr{E}_{223} & \sqrt{2}\mathscr{E}_{212} \\ \mathscr{E}_{311} & \mathscr{E}_{322} & \mathscr{E}_{333} & \sqrt{2}\mathscr{E}_{313} & \sqrt{2}\mathscr{E}_{323} & \sqrt{2}\mathscr{E}_{312} \end{bmatrix}}_{[\mathscr{E}]} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\varepsilon_{13} \\ \sqrt{2}\varepsilon_{23} \\ \sqrt{2}\varepsilon_{12} \end{bmatrix}. \tag{A.34}$$

Appendix B
Variational Calculus

The Gâteaux derivative (directional derivative, or sometimes called variation) is a generalization of the concept of directional derivative in differential calculus. In the context of the finite element method, the Gâteaux derivative is a very useful tool to derive the weak forms and linearized operators in linearized weak formulations (see e.g., Sect. 3.5 in Chap. 3, Sect. 9.1.1 in Chap. 9). Let $F(\mathbf{u})$ be a smooth vector-valued operator. The Gâteaux derivative $D_{\delta\mathbf{u}}F(\mathbf{u})$ of F at $\mathbf{u}$ in the direction $\delta\mathbf{u}$ is defined as

$$D_{\delta\mathbf{u}}F(\mathbf{u}) = \left[\frac{d}{d\alpha}F(\mathbf{u}+\alpha\delta\mathbf{u})\right]_{\alpha=0}, \tag{B.1}$$

where α is a scalar parameter. As a first example, we consider the linear gradient operator $\nabla(\mathbf{u})$. Applying the above definition, the Gâteaux derivative of the gradient operator is expressed as

$$\begin{aligned} D_{\delta\mathbf{u}}\left[\nabla(\mathbf{u})\right] &= \left[\frac{d}{d\alpha}\nabla\left(\mathbf{u}+\alpha\delta\mathbf{u}\right)\right]_{\alpha=0} = \left[\frac{d}{d\alpha}\left(\nabla\mathbf{u}+\alpha\nabla\delta\mathbf{u}\right)\right]_{\alpha=0} \\ &= \left[\nabla(\delta\mathbf{u})\right]_{\alpha=0} = \nabla(\delta\mathbf{u}). \end{aligned} \tag{B.2}$$

Then

$$\boxed{D_{\delta\mathbf{u}}\left[\nabla(\mathbf{u})\right] = \nabla(\delta\mathbf{u}).} \tag{B.3}$$

Using the previous result, let us express the Gâteaux derivative of the symmetric gradient operator $\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}\left(\nabla(\mathbf{u}) + \nabla^T(\mathbf{u})\right)$:

$$D_{\delta\mathbf{u}}\left[\varepsilon(\mathbf{u})\right] = D_{\delta\mathbf{u}}\left[\frac{1}{2}\left(\nabla\mathbf{u}+\nabla\mathbf{u}^T\right)\right] = \frac{1}{2}\left(\nabla\delta\mathbf{u}+\nabla\delta\mathbf{u}^T\right). \tag{B.4}$$

Then

$$\boxed{D_{\delta\mathbf{u}}\left[\varepsilon(\mathbf{u})\right] = \varepsilon(\delta\mathbf{u}).} \tag{B.5}$$

J. Yvonnet, *Computational Homogenization of Heterogeneous Materials with Finite Elements*, Solid Mechanics and Its Applications 258,
https://doi.org/10.1007/978-3-030-18383-7

More generally, the Gâteaux derivative has the following property when applied to linear operators. Let $\mathscr{L}$ a linear operator (see Sect. 3.4.1) then

$$\boxed{D_{\delta\mathbf{u}}\left\{\mathscr{L}\left(F\left(\mathbf{u}\right)\right)\right\} = \mathscr{L}\left(D_{\delta\mathbf{u}}F(\mathbf{u})\right).} \tag{B.6}$$

For example, Let the us consider the linear integral operator:

$$\mathscr{L}(.) = \int_{\Omega}(.)d\Omega. \tag{B.7}$$

Then

$$\begin{aligned} D_{\delta\mathbf{u}}\left[\int_{\Omega}F(\mathbf{u})d\Omega\right] &= \left[\frac{d}{d\alpha}\int_{\Omega}F(\mathbf{u}+\alpha\delta\mathbf{u})d\Omega\right]_{\alpha=0} \\ &= \int_{\Omega}\frac{d}{d\alpha}\left[F(\mathbf{u}+\alpha\delta\mathbf{u})\right]_{\alpha=0}d\Omega = \int_{\Omega}D_{\delta\mathbf{u}}F(\mathbf{u})d\Omega. \end{aligned} \tag{B.8}$$

Another property is given as follows: let F and G be two general operators, then the Gâteaux derivative verifies:

$$\boxed{D_{\delta\mathbf{u}}\left\{F(\mathbf{u})G(\mathbf{u})\right\} = \left(D_{\delta\mathbf{u}}F(\mathbf{u})\right)G(\mathbf{u}) + F(\mathbf{u})\left(D_{\delta\mathbf{u}}G(\mathbf{u})\right).} \tag{B.9}$$

As an illustrative example, we express the Gâteaux derivative of the nonlinear operator $\nabla^T(\mathbf{u})\nabla(\mathbf{u})$:

$$\begin{aligned} D_{\delta\mathbf{u}}\left\{\nabla(\mathbf{u})^T\nabla(\mathbf{u})\right\} &= \left[\frac{d}{d\alpha}\left[\nabla(\mathbf{u}+\alpha\delta\mathbf{u})^T\nabla(\mathbf{u}+\alpha\delta\mathbf{u})\right]\right]_{\alpha=0} \\ &= \left[\frac{d}{d\alpha}\left[\nabla\mathbf{u}^T\nabla\mathbf{u} + \alpha\nabla\mathbf{u}^T\nabla\delta\mathbf{u} + \alpha\nabla\delta\mathbf{u}^T\nabla\mathbf{u} + \alpha^2\nabla\delta\mathbf{u}^T\nabla\delta\mathbf{u}\right]\right]_{\alpha=0} \\ &= \left[\nabla\mathbf{u}^T\nabla\delta\mathbf{u} + \nabla\delta\mathbf{u}^T\nabla\mathbf{u} + 2\alpha\nabla\delta\mathbf{u}^T\nabla\delta\mathbf{u}\right]_{\alpha=0} \\ &= \nabla\mathbf{u}^T\nabla\delta\mathbf{u} + \nabla\delta\mathbf{u}^T\nabla\mathbf{u} = D_{\delta\mathbf{u}}\left(\nabla^T\mathbf{u}\right)\nabla\mathbf{u} + \nabla^T\mathbf{u}D_{\delta\mathbf{u}}\left(\nabla\mathbf{u}\right). \end{aligned}$$

Finally, another useful property of the Gâteaux derivative is the chain rule, given by

$$\boxed{D_{\delta\mathbf{u}}\left\{F\left(G\left(\mathbf{u}\right)\right)\right\} = \frac{\partial F}{\partial G}D_{\delta\mathbf{u}}G(\mathbf{u}).} \tag{B.10}$$

For example, if $\mathbf{G}$ is a vector-valued operator and F a scalar-valued operator, then

$$D_{\delta\mathbf{u}}\left\{F\left(\mathbf{G}\left(\mathbf{u}\right)\right)\right\} = \frac{dF}{d\mathbf{G}}\cdot D_{\delta\mathbf{u}}\mathbf{G}(\mathbf{u}) = \frac{dF}{dG_i}D_{\delta\mathbf{u}}G_i(\mathbf{u}). \tag{B.11}$$

If $\mathbf{F}$ and $\mathbf{G}$ are second-order tensor valued operators, then

$$(D_{\delta \mathbf{u}} \{\mathbf{F}(\mathbf{G}(\mathbf{u}))\})_{ij} = \left(\frac{d\mathbf{F}}{d\mathbf{G}} : D_{\delta \mathbf{u}}\mathbf{G}(\mathbf{u})\right)_{ij} = \frac{dF_{ij}}{dG_{kl}} D_{\delta \mathbf{u}} G_{kl}(\mathbf{u}). \tag{B.12}$$

In what follows, we provide the Gâteaux derivative, or variation of the strain energy density function in linear elasticity $w = \frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon}$. Using the above property, we have

$$D_{\delta \mathbf{u}} \left\{\frac{1}{2}\varepsilon(\mathbf{u}) : \mathbb{C} : \varepsilon(\mathbf{u})\right\} = \frac{1}{2}\{D_{\delta \mathbf{u}}\varepsilon(\mathbf{u}) : \mathbb{C} : \varepsilon(\mathbf{u}) + \varepsilon(\mathbf{u}) : \mathbb{C} : D_{\delta \mathbf{u}}\varepsilon(\mathbf{u})\} \tag{B.13}$$

$$= D_{\delta \mathbf{u}}\varepsilon(\mathbf{u}) : \mathbb{C} : \varepsilon(\mathbf{u}) \tag{B.14}$$

which leads to

$$D_{\delta \mathbf{u}} \left\{\frac{1}{2}\varepsilon(\mathbf{u}) : \mathbb{C} : \varepsilon(\mathbf{u})\right\} = \varepsilon(\delta \mathbf{u}) : \mathbb{C} : \varepsilon(\mathbf{u}). \tag{B.15}$$

As a last example, we apply the different above properties to compute the Gâteaux derivative, or variation, of the total elastic strain energy $E = \int_{\Omega} \omega(\boldsymbol{\varepsilon}) d\Omega$ of an elastic solid defined in a domain $\Omega \subset \mathbb{R}^3$, and for a possible nonlinear strain density function $\omega(\boldsymbol{\varepsilon})$ such that

$$\frac{\partial \omega(\varepsilon(\mathbf{u}))}{\partial \varepsilon} = \sigma(\mathbf{u}). \tag{B.16}$$

We have

$$D_{\delta \mathbf{u}} \left\{\int_{\Omega} \omega(\varepsilon(\mathbf{u}))\right\} = \int_{\Omega} D_{\delta \mathbf{u}} \{\omega[\varepsilon(\mathbf{u})]\} d\Omega$$

$$= \int_{\Omega} \frac{\partial \omega}{\partial \varepsilon} : D_{\delta \mathbf{u}}\varepsilon(\mathbf{u}) d\Omega = \int_{\Omega} \sigma(\varepsilon(\mathbf{u})) : \varepsilon(\delta \mathbf{u}) d\Omega.$$

$$= \int_{\Omega} \frac{\partial \omega(\varepsilon(\mathbf{u}))}{\partial \varepsilon} : \varepsilon(\delta \mathbf{u}) d\Omega = \int_{\Omega} \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) d\Omega. \tag{B.17}$$

Appendix C
Strain Gradient Tensors and Related Properties

C.1 Second Gradient of Displacements and Strain-Gradient Tensors

The third-order, second gradient of displacements tensor is defined as

$$\mathscr{A}_{ijk} = \frac{\partial^2 u_i}{\partial x_j \partial x_k} \tag{C.1}$$

while the third-order strain gradient tensor is defined by

$$\nabla \varepsilon_{ijk} = \frac{\partial}{\partial x_k}\left(\varepsilon_{ij}\right) = \frac{1}{2}\frac{\partial}{\partial x_k}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = \frac{1}{2}\left(\frac{\partial^2 u_i}{\partial x_j \partial x_k} + \frac{\partial^2 u_j}{\partial x_i \partial x_k}\right).$$

The relation between these two tensors can be established as follows:

$$\begin{aligned}
\mathscr{A}_{ijk} &= \frac{\partial^2 u_i}{\partial x_j \partial x_k} \\
&= \frac{1}{2}\left(\frac{\partial^2 u_i}{\partial x_j \partial x_k} + \frac{\partial^2 u_i}{\partial x_j \partial x_k} + \frac{\partial^2 u_j}{\partial x_i \partial x_k} - \frac{\partial^2 u_j}{\partial x_i \partial x_k} + \frac{\partial^2 u_k}{\partial x_i \partial x_j} - \frac{\partial^2 u_k}{\partial x_i \partial x_j}\right) \\
&= \frac{1}{2}\left(\frac{\partial^2 u_i}{\partial x_j \partial x_k} + \frac{\partial^2 u_j}{\partial x_i \partial x_k} + \frac{\partial^2 u_i}{\partial x_k \partial x_j} + \frac{\partial^2 u_k}{\partial x_i \partial x_j} - \frac{\partial^2 u_j}{\partial x_k \partial x_i} - \frac{\partial^2 u_k}{\partial x_j \partial x_i}\right) \\
&= \frac{1}{2}\left(\frac{\partial^2 u_i}{\partial x_j \partial x_k} + \frac{\partial^2 u_j}{\partial x_i \partial x_k}\right) + \frac{1}{2}\left(\frac{\partial^2 u_i}{\partial x_k \partial x_j} + \frac{\partial^2 u_k}{\partial x_i \partial x_j}\right) - \frac{1}{2}\left(\frac{\partial^2 u_j}{\partial x_k \partial x_i} - \frac{\partial^2 u_k}{\partial x_j \partial x_i}\right) \\
&= \nabla \varepsilon_{ijk} + \nabla \varepsilon_{ikj} - \nabla \varepsilon_{jki}.
\end{aligned} \tag{C.2}$$

J. Yvonnet, *Computational Homogenization of Heterogeneous Materials with Finite Elements*, Solid Mechanics and Its Applications 258,
https://doi.org/10.1007/978-3-030-18383-7

C.2 Additional Properties

We introduce the triple contraction of indices for two third order tensors $\mathscr{A}$ and $\mathscr{B}$ as: $\mathscr{A} \vdots \mathscr{B} = A_{ijk}B_{ijk}$. Let $\mathscr{A}$ be a third-order tensor and $\mathbf{B}$ a second-order tensor, then

$$\nabla \cdot (\mathscr{A} : \mathbf{B}) = (\nabla \cdot \mathscr{A}) : \mathbf{B} + \mathscr{A} \vdots \nabla\mathbf{B},$$

or

$$\frac{\partial}{\partial x_k}\left(A_{ijk}B_{jk}\right) = \frac{\partial A_{ijk}}{\partial x_k}B_{jk} + A_{ijk}\frac{\partial B_{jk}}{\partial x_k}. \tag{C.3}$$

We then introduce the following relations obtained from the divergence theorem:

$$\int_{\Omega} \nabla \cdot (\mathscr{A} : \mathbf{B})\, d\Omega = \int_{\partial\Omega} \mathbf{n} \cdot \mathscr{A} : \mathbf{B} d\Gamma. \tag{C.4}$$

or

$$\int_{\Omega} \left(\mathscr{A}_{ijk}B_{jk}\right)_{,i} d\Omega = \int_{\partial\Omega} n_i \mathscr{A}_{ijk}B_{jk} d\Gamma. \tag{C.5}$$

C.3 Quadratic Boundary Conditions

We can show that the displacement field compatible with a linear strain field in the form

$$\varepsilon_{ij}(\mathbf{x}) = \overline{\nabla\varepsilon}_{ijk}x_k \tag{C.6}$$

is given by:

$$u_i = \frac{1}{2}\overline{\mathscr{A}}_{ijk}x_j x_k, \tag{C.7}$$

as shown below. Starting from

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{C.8}$$

and using (C.2), we have

$$\frac{\partial u_i}{\partial x_j} = \frac{1}{2}\overline{\mathscr{A}}_{ipq}\left(\delta_{pj}x_q + x_p\delta_{qj}\right) = \frac{1}{2}\left(\overline{\mathscr{A}}_{ijq}x_q + \overline{\mathscr{A}}_{ipj}x_p\right) \tag{C.9}$$

$$\frac{\partial u_j}{\partial x_i} = \frac{1}{2}\overline{\mathscr{A}}_{jpq}\left(\delta_{pi}x_q + xp\delta_{qi}\right) = \frac{1}{2}\left(\overline{\mathscr{A}}_{jiq}x_q + \overline{\mathscr{A}}_{jpi}x_p\right). \tag{C.10}$$

Note that from (C.1), $\overline{\mathscr{A}}_{ijp} \neq \overline{\mathscr{A}}_{jip}$ but $\overline{\mathscr{A}}_{ijp} = \overline{\mathscr{A}}_{ipj}$. Then

$$\varepsilon_{ij} = \frac{1}{2}\left(\overline{\mathscr{A}}_{ijp} x_p + \overline{\mathscr{A}}_{jpi} x_p\right). \tag{C.11}$$

Using (C.2) and $\overline{\nabla\varepsilon}_{ijp} = \overline{\nabla\varepsilon}_{jip}$

$$\varepsilon_{ij} = \frac{1}{2}\left(\overline{\nabla\varepsilon}_{ijp} + \overline{\nabla\varepsilon}_{ipj} - \overline{\nabla\varepsilon}_{jpi} + \overline{\nabla\varepsilon}_{jip} + \overline{\nabla\varepsilon}_{jpi} - \overline{\nabla\varepsilon}_{ipj}\right) x_p = \overline{\nabla\varepsilon}_{ijp} x_p. \tag{C.12}$$

On the contrary, the choice

$$u_i = \frac{1}{2}\overline{\nabla\varepsilon}_{ijk} x_j x_k \tag{C.13}$$

does not lead to the strain field (C.6), as shown in the following:

$$\frac{\partial u_i}{\partial x_p} = \frac{1}{2}\overline{\nabla\varepsilon}_{ijk}\left(\delta_{jp} x_k + x_j \delta_{kp}\right) = \frac{1}{2}\left(\overline{\nabla\varepsilon}_{ipk} x_k + \overline{\nabla\varepsilon}_{ijp} x_j\right), \tag{C.14}$$

$$\frac{\partial u_p}{\partial x_i} = \frac{1}{2}\overline{\nabla\varepsilon}_{pjk}\left(\delta_{ji} x_k + x_j \delta_{ki}\right) = \frac{1}{2}\left(\overline{\nabla\varepsilon}_{pik} x_k + \overline{\nabla\varepsilon}_{pji} x_j\right) \tag{C.15}$$

and

$$\varepsilon_{ip} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_p} + \frac{\partial u_p}{\partial x_i}\right) \tag{C.16}$$

$$= \frac{1}{4}\left(\overline{\nabla\varepsilon}_{ipk} x_k + \overline{\nabla\varepsilon}_{ijp} x_j + \overline{\nabla\varepsilon}_{pik} x_k + \overline{\nabla\varepsilon}_{pji} x_j\right) \tag{C.17}$$

$$= \frac{1}{2}\left(\overline{\nabla\varepsilon}_{ipk} x_k\right) + \frac{1}{4}\left(\overline{\nabla\varepsilon}_{ijp} x_j + \overline{\nabla\varepsilon}_{jpi} x_j\right) \neq \overline{\nabla\varepsilon}_{ipk} x_k. \tag{C.18}$$