1 Derivatives of the Piola mapping

1.1 First-order derivatives

If we have a mapping $\mathcal{F} : \widehat{\Omega} \to \Omega$, where $\boldsymbol{\xi} \in \widehat{\Omega}$ and $\mathbf{x} \in \Omega$ are the parametric and physical coordinates, respectively, then its Jacobi-matrix is defined as

$$\mathbf{J} = \begin{bmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{bmatrix} \qquad \text{or} \qquad \mathbf{J} = \begin{bmatrix} x_\xi & x_\eta & x_\zeta \\ y_\xi & y_\eta & y_\zeta \\ z_\xi & z_\eta & z_\zeta \end{bmatrix} \tag{1}$$

We denote the Jacobian as $J = \det(\mathbf{J})$, and it is given by the determinant formula:

$$J = \begin{cases} x_\xi y_\eta - x_\eta y_\xi & , \quad \boldsymbol{\xi} = (\xi, \eta) \\ x_\xi(y_\eta z_\zeta - y_\zeta z_\eta) - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi) + x_\zeta(y_\xi z_\eta - y_\eta z_\xi) & , \quad \boldsymbol{\xi} = (\xi, \eta, \zeta) \end{cases} \tag{2}$$

From the general inversion matrix formula using the transpose of cofactor matrices, we can define the inverse of the Jacobi-matrix in two ways:

$$\mathbf{J}^{-1} = \begin{cases} \begin{bmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{bmatrix} = \frac{1}{J} \begin{bmatrix} y_\eta & -x_\eta \\ -y_\xi & x_\xi \end{bmatrix} & , \quad \boldsymbol{\xi} = (\xi, \eta) \\ \begin{bmatrix} \xi_x & \xi_y & \xi_z \\ \eta_x & \eta_y & \eta_z \\ \zeta_x & \zeta_y & \zeta_z \end{bmatrix} = \frac{1}{J} \begin{bmatrix} \begin{vmatrix} y_\eta & y_\zeta \\ z_\eta & z_\zeta \end{vmatrix} & -\begin{vmatrix} x_\eta & x_\zeta \\ z_\eta & z_\zeta \end{vmatrix} & \begin{vmatrix} x_\eta & x_\zeta \\ y_\eta & y_\zeta \end{vmatrix} \\ -\begin{vmatrix} y_\xi & y_\zeta \\ z_\xi & z_\zeta \end{vmatrix} & \begin{vmatrix} x_\xi & x_\zeta \\ z_\xi & z_\zeta \end{vmatrix} & -\begin{vmatrix} x_\xi & x_\zeta \\ y_\xi & y_\zeta \end{vmatrix} \\ \begin{vmatrix} y_\xi & y_\eta \\ z_\xi & z_\eta \end{vmatrix} & -\begin{vmatrix} x_\xi & x_\eta \\ z_\xi & z_\eta \end{vmatrix} & \begin{vmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{vmatrix} \end{bmatrix} & , \quad \boldsymbol{\xi} = (\xi, \eta, \zeta) \end{cases} \tag{3}$$

From the chain rule, we have a universal formula for the total derivative:

$$\nabla_x f = \begin{bmatrix} f_x \\ f_y \end{bmatrix} = \begin{bmatrix} f_\xi \xi_x + f_\eta \eta_x \\ f_\xi \xi_y + f_\eta \eta_y \end{bmatrix} = \begin{bmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{bmatrix} \begin{bmatrix} f_\xi \\ f_\eta \end{bmatrix} = \mathbf{J}^{-T} \nabla_\xi f \quad , \quad \boldsymbol{\xi} = (\xi, \eta) \tag{4a}$$

$$\nabla_x f = \begin{bmatrix} f_x \\ f_y \\ f_z \end{bmatrix} = \begin{bmatrix} f_\xi \xi_x + f_\eta \eta_x + f_\zeta \zeta_x \\ f_\xi \xi_y + f_\eta \eta_y + f_\zeta \zeta_y \\ f_\xi \xi_z + f_\eta \eta_z + f_\zeta \zeta_z \end{bmatrix} = \begin{bmatrix} \xi_x & \eta_x & \zeta_x \\ \xi_y & \eta_y & \zeta_y \\ \xi_z & \eta_z & \zeta_z \end{bmatrix} \begin{bmatrix} f_\xi \\ f_\eta \\ f_\zeta \end{bmatrix} = \mathbf{J}^{-T} \nabla_\xi f \quad , \quad \boldsymbol{\xi} = (\xi, \eta, \zeta) \tag{4b}$$

The Piola mapping is defined as $\mathbf{J}/J$. Its first-order derivatives are

$$\frac{\partial}{\partial x_i} \left[\frac{1}{J} \mathbf{J} \right] = -\frac{J_{x_i}}{J^2} \mathbf{J} + \frac{1}{J} \mathbf{J}_{x_i} \qquad , \qquad x_i = \{x, y, z\} \tag{5}$$

In 2D ($x_i = \{x, y\}$), the components of the first-order derivatives are

$$\mathbf{J}_{x_i} = \mathbf{J}_\xi \xi_{x_i} + \mathbf{J}_\eta \eta_{x_i} \tag{6a}$$
$$J_{x_i} = J_\xi \xi_{x_i} + J_\eta \eta_{x_i} \tag{6b}$$
$$J_\xi = (x_\xi y_\eta - x_\eta y_\xi)_\xi \tag{6c}$$
$$J_\eta = (x_\xi y_\eta - x_\eta y_\xi)_\eta \tag{6d}$$

Likewise, in 3D ($x_i = \{x, y, z\}$), the components of the first-order derivatives are

$$\mathbf{J}_{x_i} = \mathbf{J}_\xi \xi_{x_i} + \mathbf{J}_\eta \eta_{x_i} + \mathbf{J}_\zeta \zeta_{x_i} \tag{7a}$$
$$J_{x_i} = J_\xi \xi_{x_i} + J_\eta \eta_{x_i} + J_\zeta \zeta_{x_i} \tag{7b}$$
$$\begin{aligned} J_\xi = {} & x_{\xi\xi}(y_\eta z_\zeta - y_\zeta z_\eta) + x_\xi (y_\eta z_\zeta - y_\zeta z_\eta)_\xi - x_{\xi\eta}(y_\xi z_\zeta - y_\zeta z_\xi) \\ & - x_\eta (y_\xi z_\zeta - y_\zeta z_\xi)_\xi + x_{\xi\zeta}(y_\xi z_\eta - y_\eta z_\xi) + x_\zeta (y_\xi z_\eta - y_\eta z_\xi)_\xi \end{aligned} \tag{7c}$$
$$\begin{aligned} J_\eta = {} & x_{\xi\eta}(y_\eta z_\zeta - y_\zeta z_\eta) + x_\xi (y_\eta z_\zeta - y_\zeta z_\eta)_\eta - x_{\eta\eta}(y_\xi z_\zeta - y_\zeta z_\xi) \\ & - x_\eta (y_\xi z_\zeta - y_\zeta z_\xi)_\eta + x_{\eta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + x_\zeta (y_\xi z_\eta - y_\eta z_\xi)_\eta \end{aligned} \tag{7d}$$
$$\begin{aligned} J_\zeta = {} & x_{\xi\zeta}(y_\eta z_\zeta - y_\zeta z_\eta) + x_\xi (y_\eta z_\zeta - y_\zeta z_\eta)_\zeta - x_{\eta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi) \\ & - x_\eta (y_\xi z_\zeta - y_\zeta z_\xi)_\zeta + x_{\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + x_\zeta (y_\xi z_\eta - y_\eta z_\xi)_\zeta \end{aligned} \tag{7e}$$

Imagine now that we have a vector function on the form

$$\begin{bmatrix} u \\ v \end{bmatrix} = \frac{1}{J}\mathbf{J} \begin{bmatrix} \widehat{u} \\ \widehat{v} \end{bmatrix} \qquad \text{or} \qquad \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \frac{1}{J}\mathbf{J} \begin{bmatrix} \widehat{u} \\ \widehat{v} \\ \widehat{w} \end{bmatrix}$$

By using the product rule, we obtain

$$\begin{bmatrix} u \\ v \end{bmatrix}_{x_i} = \left(-\frac{J_{x_i}}{J^2}\mathbf{J} + \frac{1}{J}\mathbf{J}_{x_i} \right) \begin{bmatrix} \widehat{u} \\ \widehat{v} \end{bmatrix} + \frac{1}{J}\mathbf{J} \begin{bmatrix} \widehat{u}_\xi & \widehat{u}_\eta \\ \widehat{v}_\xi & \widehat{v}_\eta \end{bmatrix} \begin{bmatrix} \xi \\ \eta \end{bmatrix}_{x_i} \tag{8a}$$
$$\begin{bmatrix} u \\ v \\ w \end{bmatrix}_{x_i} = \left(-\frac{J_{x_i}}{J^2}\mathbf{J} + \frac{1}{J}\mathbf{J}_{x_i} \right) \begin{bmatrix} \widehat{u} \\ \widehat{v} \\ \widehat{w} \end{bmatrix} + \frac{1}{J}\mathbf{J} \begin{bmatrix} \widehat{u}_\xi & \widehat{u}_\eta & \widehat{u}_\zeta \\ \widehat{v}_\xi & \widehat{v}_\eta & \widehat{v}_\zeta \\ \widehat{w}_\xi & \widehat{w}_\eta & \widehat{w}_\zeta \end{bmatrix} \begin{bmatrix} \xi \\ \eta \\ \zeta \end{bmatrix}_{x_i} \tag{8b}$$

1.2 Second-order derivatives

From the double product rule, the second-order derivative is given by

$$\left[\frac{1}{J}\mathbf{J}\right]_{x_i x_i} = \left[-\frac{J_{x_i x_i}}{J^2} + \frac{2J_{x_i}^2}{J^3} \right] \mathbf{J} - 2\frac{J_{x_i}}{J^2}\mathbf{J}_{x_i} + \frac{1}{J}\mathbf{J}_{x_i x_i} \qquad , \qquad x_i = \{x, y, z\} \tag{9}$$

As we see from these formulas, the real objective is finding J_{xx}, J_{yy}, J_{zz}, $\mathbf{J}_{xx}$, $\mathbf{J}_{yy}$ and $\mathbf{J}_{zz}$. We start with $\mathbf{J}$ and use the total derivative rule:

$$\mathbf{J}_{x_i x_i} = (\mathbf{J}_{\xi\xi}\xi_{x_i} + \mathbf{J}_{\xi\eta}\eta_{x_i})\xi_{x_i} + \mathbf{J}_\xi \xi_{x_i x_i} + (\mathbf{J}_{\xi\eta}\xi_{x_i} + \mathbf{J}_{\eta\eta}\eta_{x_i})\eta_{x_i} + \mathbf{J}_\eta \eta_{x_i x_i} \tag{10a}$$
$$\begin{aligned} \mathbf{J}_{x_i x_i} = {} & (\mathbf{J}_{\xi\xi}\xi_{x_i} + \mathbf{J}_{\xi\eta}\eta_{x_i} + \mathbf{J}_{\xi\zeta}\zeta_{x_i})\xi_{x_i} + \mathbf{J}_\xi \xi_{x_i x_i} + (\mathbf{J}_{\xi\eta}\xi_{x_i} + \mathbf{J}_{\eta\eta}\eta_{x_i} + \mathbf{J}_{\eta\zeta}\zeta_{x_i})\eta_{x_i} \\ & + \mathbf{J}_\eta \eta_{x_i x_i} + (\mathbf{J}_{\xi\zeta}\xi_{x_i} + \mathbf{J}_{\eta\zeta}\eta_{x_i} + \mathbf{J}_{\zeta\zeta}\zeta_{x_i})\zeta_{x_i} + \mathbf{J}_\zeta \zeta_{x_i x_i} \end{aligned} \tag{10b}$$

In 2D ($x_i = \{x, y\}$), the second-order derivative determinants become

$$
\begin{align}
J_{x_i x_i} &= \left(J_{\xi\xi}\xi_{x_i} + J_{\xi\eta}\eta_{x_i}\right)\xi_{x_i} + J_\xi \xi_{x_i x_i} + \left(J_{\xi\eta}\xi_{x_i} + J_{\eta\eta}\eta_{x_i}\right)\eta_{x_i} + J_\eta \eta_{x_i x_i} \tag{11a}\\
J_{\xi\xi} &= (x_\xi y_\eta - x_\eta y_\xi)_{\xi\xi} \tag{11b}\\
J_{\xi\eta} &= (x_\xi y_\eta - x_\eta y_\xi)_{\xi\eta} \tag{11c}\\
J_{\eta\eta} &= (x_\xi y_\eta - x_\eta y_\xi)_{\eta\eta} \tag{11d}
\end{align}
$$

Likewise, in 3D ($x_i = \{x, y, z\}$), the second-order derivative determinants become

$$
\begin{align}
J_{x_i x_i} &= \left(J_{\xi\xi}\xi_{x_i} + J_{\xi\eta}\eta_{x_i} + J_{\xi\zeta}\zeta_{x_i}\right)\xi_{x_i} + J_\xi \xi_{x_i x_i} + \left(J_{\xi\eta}\xi_{x_i} + J_{\eta\eta}\eta_{x_i} + J_{\eta\zeta}\zeta_{x_i}\right)\eta_{x_i} \nonumber\\
&\quad + J_\eta \eta_{x_i x_i} + \left(J_{\xi\zeta}\xi_{x_i} + J_{\eta\zeta}\eta_{x_i} + J_{\zeta\zeta}\zeta_{x_i}\right)\zeta_{x_i} + J_\zeta \zeta_{x_i x_i} \tag{12a}\\
J_{\xi\xi} &= x_{\xi\xi\xi}(y_\eta z_\zeta - y_\zeta z_\eta) + 2x_{\xi\xi}(y_\eta z_\zeta - y_\zeta z_\eta)_\xi + x_\xi(y_\eta z_\zeta - y_\zeta z_\eta)_{\xi\xi} \nonumber\\
&\quad - x_{\xi\xi\eta}(y_\xi z_\zeta - y_\zeta z_\xi) - 2x_{\xi\eta}(y_\xi z_\zeta - y_\zeta z_\xi)_\xi - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi)_{\xi\xi} \nonumber\\
&\quad + x_{\xi\xi\zeta}(y_\xi z_\eta - y_\eta z_\xi) + 2x_{\xi\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\xi + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)_{\xi\xi} \tag{12b}\\
J_{\eta\eta} &= x_{\xi\eta\eta}(y_\eta z_\zeta - y_\zeta z_\eta) + 2x_{\xi\eta}(y_\eta z_\zeta - y_\zeta z_\eta)_\eta + x_\xi(y_\eta z_\zeta - y_\zeta z_\eta)_{\eta\eta} \nonumber\\
&\quad - x_{\eta\eta\eta}(y_\xi z_\zeta - y_\zeta z_\xi) - 2x_{\eta\eta}(y_\xi z_\zeta - y_\zeta z_\xi)_\eta - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi)_{\eta\eta} \nonumber\\
&\quad + x_{\eta\eta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + 2x_{\eta\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\eta + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)_{\eta\eta} \tag{12c}\\
J_{\zeta\zeta} &= x_{\xi\zeta\zeta}(y_\eta z_\zeta - y_\zeta z_\eta) + 2x_{\xi\zeta}(y_\eta z_\zeta - y_\zeta z_\eta)_\zeta + x_\xi(y_\eta z_\zeta - y_\zeta z_\eta)_{\zeta\zeta} \nonumber\\
&\quad - x_{\eta\zeta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi) - 2x_{\eta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi)_\zeta - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi)_{\zeta\zeta} \nonumber\\
&\quad + x_{\zeta\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + 2x_{\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\zeta + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)_{\zeta\zeta} \tag{12d}\\
J_{\xi\eta} &= x_{\xi\xi\eta}(y_\eta z_\zeta - y_\zeta z_\eta) + x_{\xi\xi}(y_\eta z_\zeta - y_\zeta z_\eta)_\eta + x_{\xi\eta}(y_\eta z_\zeta - y_\zeta z_\eta)_\xi + x_\xi(y_\eta z_\zeta - y_\zeta z_\eta)_{\eta\eta} \nonumber\\
&\quad - x_{\xi\eta\eta}(y_\xi z_\zeta - y_\zeta z_\xi) - x_{\xi\eta}(y_\xi z_\zeta - y_\zeta z_\xi)_\eta - x_{\eta\eta}(y_\xi z_\zeta - y_\zeta z_\xi)_\xi - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi)_{\xi\eta} \nonumber\\
&\quad + x_{\xi\eta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + x_{\xi\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\eta + x_{\eta\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\xi + x_\zeta(y_\xi z_\eta - y_\eta z_{\xi\xi\eta}) \tag{12e}\\
J_{\xi\zeta} &= x_{\xi\xi\zeta}(y_\eta z_\zeta - y_\zeta z_\eta) + x_{\xi\xi}(y_\eta z_\zeta - y_\zeta z_\eta)_\zeta + x_{\xi\zeta}(y_\eta z_\zeta - y_\zeta z_\eta)_\xi + x_\xi(y_\eta z_\zeta - y_\zeta z_\eta)_{\xi\zeta} \nonumber\\
&\quad - x_{\xi\eta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi) - x_{\xi\eta}(y_\xi z_\zeta - y_\zeta z_\xi)_\zeta - x_{\eta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi)_\xi - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi)_{\xi\zeta} \nonumber\\
&\quad + x_{\xi\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + x_{\xi\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\zeta + x_{\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\xi + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)_{\xi\zeta} \tag{12f}\\
J_{\eta\zeta} &= x_{\xi\eta\zeta}(y_\eta z_\zeta - y_\zeta z_\eta) + x_{\xi\eta}(y_\eta z_\zeta - y_\zeta z_\eta)_\zeta + x_{\xi\zeta}(y_\eta z_\zeta - y_\zeta z_\eta)_\eta + x_\xi(y_\eta z_\zeta - y_\zeta z_\eta)_{\eta\zeta} \nonumber\\
&\quad - x_{\eta\eta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi) - x_{\eta\eta}(y_\xi z_\zeta - y_\zeta z_\xi)_\zeta - x_{\eta\zeta}(y_\xi z_\zeta - y_\zeta z_\xi)_\eta - x_\eta(y_\xi z_\zeta - y_\zeta z_\xi)_{\eta\zeta} \nonumber\\
&\quad + x_{\eta\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi) + x_{\eta\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\zeta + x_{\zeta\zeta}(y_\xi z_\eta - y_\eta z_\xi)_\eta + x_\zeta(y_\xi z_\eta - y_\eta z_\xi)_{\zeta\zeta} \tag{12g}
\end{align}
$$