4

More on Small Orientation Changes

Infinitesimally small changes of orientations are essential for rotational kinematics. They are important also in textures; especially for the analysis of texture evolution in plastic deformation of polycrystals.

4.1 Vector of Infinitesimal Rotation

Orientation changes linear in orientation parameters are usually described by a certain vector, which will be denoted here by \( \omega \). Let an orientation be represented by an orthogonal matrix \( O \). By adding small quantities grouped in the matrix \( dO \) to the entries of \( O \), we get the matrix \( O + dO \) which is orthogonal if \( dO \) satisfies

\[
O^T dO + dO^T O + dO^T dO = 0. \tag{4.1}
\]

The misorientation \( \delta O \) between \( O + dO \) and \( O \) can be written in the form

\[
\delta O = O^T (O + dO) = I + \Omega, \quad \text{where} \quad \Omega = O^T dO. \tag{4.2}
\]

For small entries of \( dO \), with the quadratic term \( dO^T dO \) in Eq.(4.1) neglected, the matrix \( \Omega \) is antisymmetric, i.e., \( \Omega + \Omega^T = 0 \). The relationship between \( \Omega \) and tangent vectors is embodied in Eq.(3.33). At the identity, the matrix \( \Omega \) is directly related to the matrices given by (3.35) \( \Omega \big|_{\text{at the identity}} = E_k d\xi^k \), where \( \xi^k \) are the rotation parameters. With antisymmetric \( \Omega \), the matrix \( \delta O \) can be expressed as

\[
\delta O_{ij} = \delta_{ij} + \varepsilon_{ijk} \omega_k, \\
\]

where \( \omega \) is the vector of infinitesimal rotation given by \( \omega_i = \varepsilon_{ijk} \Omega_{jk}/2 \).

The vector \( \omega_i \) depends linearly on infinitesimal changes of other orientation parameters. For the Rodrigues parameters \( r^i \), based on the relation (2.14), \( dO \) is given by

\[
dO_{ij} = (2/(1 + r^k r^k)^2) \left( (1 + r^m r^m)(r^i dr^j + r^j dr^i) - 2(\delta_{ij} + r^i r^j) r^m dr^m \right. \\
\left. + \varepsilon_{ijn}(2 r^m r^m dr^m - dr^n (1 + r^m r^m)) \right). \\
\]
Hence, the definition of the vector $\vec{w}$ leads to

$$\vec{w}_i = \frac{-2}{(1 + r^m r^m)} (\delta_{ik} - \varepsilon_{ijk} r^j) \, dr^k . \quad (4.3)$$

The inverse relation has the form

$$dr^i = -\frac{1}{2} (\delta_{ik} + r^i r^k + \varepsilon_{ijk} r^j) \, \vec{w}_k . \quad (4.4)$$

**Alternative derivation**

The same can be obtained by calculating components $\delta r^i$ of the Gibbs vector $\delta r = (-r) \circ (r + dr)$

$$\delta r^i = \frac{\delta_{ij} + \varepsilon_{ijk} k^k}{1 + r^l r^l} \, dr^j .$$

The orthogonal matrix $\delta O$ and the corresponding Rodrigues vector $\delta r$ are related via Eq.(2.14)

$$\delta O_{ij} = \delta_{ij} - 2\varepsilon_{ijk} \frac{\delta_{kl} + \varepsilon_{klm} r^m}{1 + r^l r^l} \, dr^i .$$

By comparing this with $\delta O_{ij} = \delta_{ij} + \varepsilon_{ijk} \vec{w}_k$, Eq.(4.3) is obtained. □

Proceeding in an analogous way, the following relations between the vector of infinitesimal rotation and the increment of quaternion coordinates $q^i$, $i = 1, 2, 3$ can be derived:

$$\vec{w}_i = \frac{-2}{q^0} \left( (q^0)^2 \delta_{ij} + q^i q^j + \varepsilon_{ijk} q^k q^0 \right) \, dq^j \quad \text{and} \quad dq^i = -\frac{1}{2} \left( q^0 \delta_{ij} - \varepsilon_{ijk} q^k \right) \vec{w}_j .$$

The first relation means that $-\vec{w}_i/2$ is the vector part of the quaternion $q^* \circ dq$ with $dq^0$ determined by $q^* \circ dq^0 = d(q^* q^0)/2 = 0$; the scalar part of $q^* \circ dq$ is zero.

Based on the relation between axis/angle parameters $(n, \omega)$ and the entries of the orthogonal matrix (Eq.2.21), we have

$$\vec{w}_i = -(n_1 d\omega + (\sin \omega \delta_{ik} - (1 - \cos \omega) \varepsilon_{ijk} n_j) d n_k) ,$$

where $n_k d n_k = d(n_k n_k)/2 = 0$. It is obvious here that in the 'axis–angle' parameterization, a change of the $n_k$ parameters corresponds to a rotation; this is not always clear, when infinitesimal rotations are defined via $n_i d\omega$ with fixed rotation axis.

The vector $\vec{w}$ and increments of Euler angles are related by

$$\begin{align*}
\vec{w}_1 &= \cos \varphi_1 \, d\phi + \sin \varphi_1 \sin \phi \, d\varphi_2 \\
\vec{w}_2 &= \sin \varphi_1 \, d\phi - \cos \varphi_1 \sin \phi \, d\varphi_2 \\
\vec{w}_3 &= d\varphi_1 + \cos \phi \, d\varphi_2
\end{align*} \quad (4.5)$$

and

$$\begin{align*}
d\varphi_1 &= -\cot \phi \sin \varphi_1 \, \vec{w}_1 + \cot \phi \cos \varphi_1 \, \vec{w}_2 + \vec{w}_3 \\
d\phi &= \cos \varphi_1 \, \vec{w}_1 + \sin \varphi_1 \, \vec{w}_2 \\
d\varphi_2 &= \csc \phi \sin \varphi_1 \, \vec{w}_1 - \csc \phi \cos \varphi_1 \, \vec{w}_2 .
\end{align*}$$