Abstract

This note outlines the steps necessary to rotate selected (nodal) coordinates using quaternions.

1. Introduction

The rotation of coordinates can be described by a rotation angle and a rotation axis. For rotations in 3-dimensional space, we introduce a 4-dimensional quaternion \( Q \) as follows:

\[
Q = (Q_0, Q_1, Q_2, Q_3) \tag{1}
\]

For a rotation axis \( \vec{n} \) and a rotation angle \( \varphi \), we can define a unit quaternion \( q \) as follows:

\[
q = \left( \cos \frac{\varphi}{2}, \hat{n} \sin \frac{\varphi}{2} \right). \tag{2}
\]

Here we introduced the normalized vector \( \hat{n} \) which belongs to \( \vec{n} \). The rotation of an arbitrary point \( \vec{r} \) about the axis \( \vec{n} \) with angle \( \varphi \) can now be described with quaternions:

\[
(0, \vec{r}') = q \ast (0, \vec{r}) \ast \bar{q} \tag{3}
\]

\( \bar{q} \) is the conjugate quaternion belonging to \( q \): \( \bar{q} = (q_0, -q_1, -q_2, -q_3) \). The unit quaternion has the property \( \bar{q} = q^{-1} \) and the following equation holds: \( 1 = q \cdot \bar{q} \). \( ( \ast ) \) denotes the quaternion product, which is being calculated from right to left. The quaternion product is defined as follows:

\[
(a, \vec{b}) \ast (c, \vec{d}) = (ac - \vec{b} \cdot \vec{d}, a \vec{d} + c \vec{b} + \vec{b} \times \vec{d}) \tag{4}
\]

Here, \( (\cdot) \) denotes the scalar product and \( (\times) \) the cross product in \( \mathbb{R}^3 \). If we now calculate the product in equation (3) with the Graßmann identity of the cross product of three vectors:

\[
(0, \vec{r}') = q \ast (0, \vec{r}) \ast \bar{q} \\
= q \ast (0, \vec{r}) \ast \left( \cos \frac{\varphi}{2}, -\hat{n} \sin \frac{\varphi}{2} \right) \\
= \left( \cos \frac{\varphi}{2}, \hat{n} \sin \frac{\varphi}{2} \right) \ast \left( \vec{r} \cdot \hat{n} \sin \frac{\varphi}{2}, \vec{r} \cos \frac{\varphi}{2} - \vec{r} \times \hat{n} \sin \frac{\varphi}{2} \right) \\
= \left( \vec{r} \left( \cos \frac{\varphi}{2} \right)^2 - \vec{r} \left( \sin \frac{\varphi}{2} \right)^2 + 2 \hat{n} (\vec{r} \cdot \hat{n}) \left( \sin \frac{\varphi}{2} \right)^2 - 2 \vec{r} \times \hat{n} \sin \frac{\varphi}{2} \frac{\cos \varphi}{2} \right) \\
= \left( \vec{r} \left( 1 - 2 \left( \sin \frac{\varphi}{2} \right)^2 \right) + 2 \hat{n} (\vec{r} \cdot \hat{n}) \left( \sin \frac{\varphi}{2} \right)^2 - 2 \vec{r} \times \hat{n} \sin \frac{\varphi}{2} \frac{\cos \varphi}{2} \right) ,
\]
we obtain the following:

\[ \vec{r}' = \vec{r} a(\varphi) + \hat{n} b(\vec{r}, \hat{n}, \varphi) + (\vec{r} \times \hat{n}) c(\varphi). \]  

(5)

The coefficients \(a, b, \) and \(c\) herein are defined as follows:

\[ a(\varphi) = 1 - 2 \left( \sin \frac{\varphi}{2} \right)^2 \]  

(6)

\[ b(\vec{r}, \hat{n}, \varphi) = 2 \vec{r} \cdot \hat{n} \left( \sin \frac{\varphi}{2} \right)^2 \]  

(7)

\[ c(\varphi) = -2 \sin \frac{\varphi}{2} \cos \frac{\varphi}{2} \]  

(8)

1.1. 2D Case

In 2 dimensions we use a simple trick. We use the settings explaind above, set the \(z\)-component of the position vector to 0 and let the axis of rotation point out of the \(xy\)-plane:

\[ \vec{r} = (x, y, 0) \]  

(9)

\[ \vec{n} = (0, 0, 1). \]  

(10)

This implies that the coefficient \(b\) is zero in the 2D case. Using the addition theorem for angles we can show that equation (5) holds for 2D as well.

2. Implementation of Coordinate Rotation

The quaternion rotation is implemented in the subroutine

\texttt{xns:update.F:updatex}. 

For the rotation one needs the rotation vector \(\omega\). The normalized rotation vector and angle can be identified with \(\hat{n}\) and \(\varphi\). In the source they are

\[
\begin{align*}
\text{ox} &= \text{omega}(\text{xsd}) \times \text{dt} \\
\text{oy} &= \text{omega}(\text{ysd}) \times \text{dt} \\
\text{oz} &= \text{omega}(\text{zsd}) \times \text{dt} \\
\text{ot} &= \text{dsqrt}((\text{ox} \times \text{ox} + \text{oy} \times \text{oy} + \text{oz} \times \text{oz})) \\
\text{ox} &= \text{ox} / \text{ot} \\
\text{oy} &= \text{oy} / \text{ot} \\
\text{oz} &= \text{oz} / \text{ot}
\end{align*}
\]

where \(\text{ox}, \text{oy}\) and \(\text{oz}\) are the components of the normalized rotation axis and \(\text{ot}\) is the angle. We determine the coefficients \textit{quata} (6), \textit{quatb} (7) and \textit{quatc} (8) and do the rotation:

\[
\begin{align*}
\text{ot} &= \text{ot} / 2.0 \text{d0} \\
\text{ct} &= \text{dcos}(\text{ot}) \\
\text{st} &= \text{dsin}(\text{ot})
\end{align*}
\]
Node Rotation with Quaternions

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\[ \text{quat}a = 1.0d0 - 2.0d0*\text{st}^2\text{st} \]
\[ \text{quat}c = -2.0d0*\text{st}^2\text{ct} \]

do inlreg=1,nlnreg

if (mlev(inl).gt.0) then

inlbot = mlev(inl)
inltop = inl

rx = x(xsd,inlbot) - cx
ry = x(ysd,inlbot) - cy
if(nsd.eq.3) rz = x(zsd,inlbot) - cz

\[ \text{quat}b = 2.0d0*\text{st}^2\text{st} \times (\text{rx}\text{ox} + \text{ry}\text{oy} + \text{rz}\text{oz}) \]

c quaternion product component-wise:

\[ \text{x}(\text{xsd},\text{inltop}) = \text{rx}\text{quat}a + \text{ox}\text{quat}b + (\text{ry}\text{oz} - \text{rz}\text{oy})*\text{quat}c + \text{cx} \]
\[ \text{x}(\text{ysd},\text{inltop}) = \text{ry}\text{quat}a + \text{oy}\text{quat}b + (\text{rz}\text{ox} - \text{rx}\text{oz})*\text{quat}c + \text{cy} \]
if (nsd.eq.3) \[ \text{x}(\text{zsd},\text{inltop}) = \text{rz}\text{quat}a + \text{oz}\text{quat}b + (\text{rx}\text{oy} - \text{ry}\text{ox})*\text{quat}c + \text{cz} \]

m(xsd,inltop) = .true.
m(ysd,inltop) = .true.
if (nsd.eq.3) m(zsd,inltop) = .true.

end if

end do.

Now, the top level coordinates are rotated relative to the bottom level coordinates.

History

August 26, 2009 Written.