Rotations in Chrono::Engine

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Abstract
This covers some theoretical aspects about rotations in 3D. The main formulas that are implemented in Chrono::Engine for handling rotations are presented in this document. Rotations are mostly dealt via quaternion algebra in Chrono::Engine, so here we also provide an introductory section on quaternions and quaternion algebra in general.

1. Quaternions

Quaternions represent the preferred method for parametrizing rotations in Chrono::Engine API.

They are implemented in the chrono::ChQuaternion class and they are used extensively through all the code. For instance they are used for expressing the rotations of rigid bodies: chrono::ChBody.

Quaternions algebra plays a fundamental role in computational mechanics as they represent a very useful tool to express rotations of coordinate systems [1, 2, 3].

Differently from other systems of parametrization based on three angles, they do not suffer problems of singularity when converted from/to a rotation matrix $A \in SO3$.

Moreover their algebra allow a compact set of formulas for rotating points, and to operate with angular velocity and angular acceleration.

For the above mentioned reasons, quaternions are widely used in the Chrono::Engine API. In the following we will report the main formulas implemented in it.
2. Elements of quaternion algebra

Quaternion algebra is a non-commutative field \( \mathbb{H}(\cdot, +) \), as such it has the neutral element and it has associative and distributive properties both for multiplication and addition, but, differently from real and complex algebras, it is commutative only respect to addition.

They are complex numbers with three imaginary units and one real unit, from the data storage point of view they are vectors with four dimensions.

Usually they are written as \( q \in \mathbb{H} = q_0, q_1, q_2, q_3 \in \mathbb{R} \):

\[
q = (q_0 + q_1 \cdot i + q_2 \cdot j + q_3 \cdot k) \tag{1}
\]

where the three imaginary units \( i, j, k \) have the following properties:

\[
i^2 = -1 \tag{2a}
\]
\[
j^2 = -1 \tag{2b}
\]
\[
k^2 = -1 \tag{2c}
\]
\[
i \cdot j \cdot k = -1 \tag{2d}
\]
\[
i \cdot j = -j \cdot i = k \tag{2e}
\]
\[
j \cdot k = -k \cdot j = i \tag{2f}
\]
\[
k \cdot i = -i \cdot k = j \tag{2g}
\]

Properties of Eq.(2) can be reassumed in Table (1) that shows the multiplication rules for the bases.

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Table 1: Rules for products among \( \{1, -1, i, -i, j, -j, k, -k\} \)

The properties above define also products and sums between quaternions.

In detail, the sum or difference between \( \mathbf{a} \in \mathbb{H} \) and \( \mathbf{b} \in \mathbb{H} \) gives a quaternion \( \mathbf{c} \in \mathbb{H} \) with this rule:

\[
\mathbf{c} = \mathbf{a} \pm \mathbf{b} =
\]
\[
= (a_0 + a_1 \cdot i + a_2 \cdot j + a_3 \cdot k) \pm (b_0 + b_1 \cdot i + b_2 \cdot j + b_3 \cdot k) =
\]
\[
= (a_0 \pm b_0) \pm (a_1 \pm b_1) \cdot i \pm (a_2 \pm b_2) \cdot j \pm (a_3 \pm b_3) \cdot k \tag{3}
\]

Note that the sum is commutative:

\[
\mathbf{a} \pm (\mathbf{b} \pm \mathbf{c}) = (\mathbf{a} \pm \mathbf{b}) \pm \mathbf{c} \tag{4a}
\]
\[
\mathbf{a} \pm \mathbf{b} = \mathbf{b} \pm \mathbf{a} \tag{4b}
\]
The product between quaternions \( a \in \mathbb{H} \) and \( b \in \mathbb{H} \) gives a quaternion \( c \in \mathbb{H} \) with the following rule:

\[
c = a \cdot b = \frac{1}{2} (a b_0 - a_1 b_1 - a_2 b_2 - a_3 b_3) + \frac{1}{2} (a_0 b_1 + a_1 b_0 + a_2 b_3 - a_3 b_2) i + \frac{1}{2} (a_0 b_2 - a_1 b_3 + a_2 b_0 + a_3 b_1) j + \frac{1}{2} (a_0 b_3 + a_1 b_2 - a_2 b_1 + a_3 b_0) k
\]  

The product is associative and distributive. Except rare cases, it is not commutative, though:

\[
a (b c) = (a b) c \quad (6a)
\]

\[
a b \neq b a \quad (6b)
\]

We also introduce the product between a quaternion and a scalar: for instance between \( q \in \mathbb{H} \) and \( s \in \mathbb{R} \) gives \( r \in \mathbb{H} \) according to:

\[
r = q s = q (s + 0i + 0j + 0k) = (s q_0 + s q_1 i + s q_2 j + s q_3 k)
\]  

This product by a scalar is commutative:

\[
a s = s a \quad (8a)
\]

\[
a 1 = 1 a \quad (8b)
\]

\[
s z a = z s a \quad (8c)
\]

\[
a (s b + z c) = s a b + z a c \quad (8d)
\]

The conjugate of a quaternion, similarly to the conjugate of a complex number, is obtained by flipping the sign of the imaginary unit:

\[
q = (q_0 + q_1 i + q_2 j + q_3 k)
\]

\[
q^* = (q_0 - q_1 i - q_2 j - q_3 k)
\]  

The following properties hold:

\[
(a^*)_* = a \quad (10a)
\]

\[
(a b)^* = b^* a^* \quad (10b)
\]

\[
(a + b)^* = a^* + b^* \quad (10c)
\]  

3
A very important property is related to the product of a quaternion by its conjugate: in such case, the result corresponds to a quaternion with only the real part:

\[
q q^* = (q_0^2 + q_1^2 + q_2^2 + q_3^2) \quad (11a)
\]

\[
q q^* = q^* q = s \in \mathbb{R} \quad (11b)
\]

Property (11) can be easily demonstrated using definitions (5) and (9).

Multiplication by a conjugate can be used also to define the norm of a quaternion, similar to the euclidean norm in \( \mathbb{R}^4 \):

\[
|q| = \sqrt{q q^*} \quad (12a)
\]

\[
|q| = \sqrt{(q_0^2 + q_1^2 + q_2^2 + q_3^2)} \quad (12b)
\]

By introducing the \(||\) norm, the quaternion algebra \( \mathbb{H}(\cdot, +, ||) \) becomes a Banach algebra, with metric space \( \mathbb{H} \).

The following properties hold:

\[
|q| \geq 0 \quad (13a)
\]

\[
|q| = 0 \iff q = (0 + 0i + 0j + 0k) \quad (13b)
\]

\[
|sq| = s|q| \quad (13c)
\]

\[
|q + r| \leq |q| + |r| \quad (13d)
\]

\[
|qr| = |q||r| \quad (13e)
\]

Quaternion algebra is a divisional algebra because for each \( q \neq 0 \), one can compute the inverse \( q^{-1} \) such that \( q^{-1} q = 1 \). In fact, since for (11) and (12) one has \( (qq^*/|q|^2) = 1 \), it is easy to demonstrate that:

\[
q^{-1} = q^* \frac{1}{|q|^2} \quad (14)
\]

In sake of computational efficiency, remember that the inverse of an unimodular quaternion is simply its conjugate:

\[
|q| = 1 \implies q^{-1} = q^* \quad (15)
\]

3. Alternative notations

It is useful to recall that, other than the notation in (1), there are other notations to express quaternions. In detail, the original notation by Hamilton puts in
evidence the so called scalar part \( s \in \mathbb{R} \) and the imaginary vectorial part \( \mathbf{v} \in \text{Im}\mathbb{H} \), with \( \mathbb{H} = \mathbb{R} \oplus \text{Im}\mathbb{H} \):

\[
\mathbf{q} = (s, \mathbf{v})
\]  

(16)

This notation \(^1\) allows a more compact expression for the addition and multiplication formulas (3) e (5):

\[
\mathbf{a} \pm \mathbf{b} = (s_a \pm s_b, \mathbf{v}_a \pm \mathbf{v}_b) \\
\mathbf{ab} = (s_a s_b - \mathbf{v}_a \cdot \mathbf{v}_b, s_a \mathbf{v}_b + s_b \mathbf{v}_a + \mathbf{v}_a \times \mathbf{v}_b)
\]  

(17a, b)

where we used the symbols of scalar product (\( \cdot \)) and of vector product (\( \times \)) as already used for vectors in \( \mathbb{R}^3 \).

A quaternion with an imaginary part only, \( \mathbf{q} = (0, \mathbf{v}) \), is said pure quaternion or imaginary, whereas a quaternion with a real part only is said real quaternion.

Another representation of quaternions can be done using column vectors with four dimensions:

\[
\mathbf{q} = \{q_0, q_1, q_2, q_3\}^T
\]

(18)

Such notation is especially useful when one wants to perform quaternion algebra using the tools of matrix multiplication as in linear algebra.

In such a context, using (5), the product between two quaternions is represented by a product of a 4x4 matrix an a 4x1 vector, as follows:

\[
\begin{bmatrix} +a_0 & -a_1 & -a_2 & -a_3 \\ +a_1 & +a_0 & -a_3 & +a_2 \\ +a_2 & +a_3 & +a_0 & -a_1 \\ +a_3 & -a_2 & +a_1 & +a_0 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix}
\]

(19)

For compactness we introduce \([M_\oplus]\) c \([M_\ominus]\):

\[
\mathbf{a} \mathbf{b} = \mathbf{c} \iff [M(a)_\oplus] \mathbf{b} = [M(b)_\ominus] \mathbf{a}
\]

(20a)

\[
[M(a)_\oplus] = \begin{bmatrix} +a_0 & -a_1 & -a_2 & -a_3 \\ +a_1 & +a_0 & -a_3 & +a_2 \\ +a_2 & +a_3 & +a_0 & -a_1 \\ +a_3 & -a_2 & +a_1 & +a_0 \end{bmatrix}
\]

(20b)

\[
[M(b)_\ominus] = \begin{bmatrix} +b_0 & -b_1 & -b_2 & -b_3 \\ +b_1 & +b_0 & +b_3 & -b_2 \\ +b_2 & -b_3 & +b_0 & +b_1 \\ +b_3 & +b_2 & -b_1 & +b_0 \end{bmatrix}
\]

(20c)

\(^1\)The \( \mathbf{q} = (s, \mathbf{v}) \) notation is especially used in computer graphics
4. Rotations

Let's consider $p \in \mathbb{H} \rightarrow p' \in \mathbb{H}$, transforming $p$ into quaternion $p'$:

$$p' = q p q^*$$

(21)

Form the property (13e) it follows that

$$|p'| = |q||p||q^*|$$

(22)

When using quaternions $q$ of unit length only, (unitary quaternions), it happens that the norm of $p$ is not modified by the transformation, as $|p'| = |q||p||q^*| = |p|1$.

Therefore when $|q| = 1$, the endomorphism (21) operates a rotation of the $p$ quaternion.

Even more interesting is the case where $p \in \text{Im}\mathbb{H}$, because in such a case, for $|q| = 1$, even the transformed quaternion has only an imaginary part: $p' \in \text{Im}\mathbb{H}$.

This means that one can use the notation (21) to express a rotation of a vector $v$ (a position of a point in three dimensional space) into a rotated vector $v'$, simply assuming $p = (0, v)$:

$$p' = q p q^*$$

$$ (0, v') = q (0, v) q^*$$

(23)

Sequences of rotations can be expressed shortly in the same way. For example, rotating $p$ in $p'$ by means of $q_a$, and later rotating $p'$ in $p''$ by means of $q_b$, one has:

$$p' = q_a p q_{a^*}$$

$$p'' = q_b p' q_{b^*}$$

$$p'' = (q_b q_a) p (q_{a^*} q_{b^*})$$

More in general, remembering (10b), given $n$ rotations expressed by $q_1, \ldots, q_n$, quaternions, one has:

$$p' = q_s p q_{s^*}$$

(24)

where $q_s = (q_n, \ldots, q_2, q_1)$.

Obviously, as quaternion multiplication is not commutative, it follows that is it not possible to change the order of the terms $q_1, \ldots, q_n$.

The inverse transformation is obtained by premultiplying the two terms of (21) by $q^*$ and by post-multiplying by $q$, obtaining $q^* p' q = q^* q p q^* q$. Given that $q^* q = qq^* = 1$, we have:

$$p' = q p q^*$$

$$p = q^* p' q$$

(25)
We looked at how (21) makes a rotation by means of two simple quaternion multiplications; it is interesting to pair this with other equivalent, maybe more classical, means of computing rotations.

For example given a rotation matrix \([A]\) for the well known transformation \(v' = [A]v\), it is often needed to find the quaternion \(q\) that makes the same rotation in \((0, v') = q(0, v)q^\ast\), or vice versa.

Therefore, we express (21) wit linear algebra, using (20). One obtains:

\[
p' = [M(q)\mathbb{E}](p q^\ast)
\]

\[
= [M(q)\mathbb{E}][M(q^\ast)\mathbb{E}]p
\]

\[
= +g_0 -q_1 -q_2 -q_3 +q_0 +q_1 +q_2 +q_3 +q_0 -q_3 +q_2 +q_1 +q_0 -q_1 -q_0 -q_1 -q_0 +q_3 -q_2 +q_1 +q_0
\]

\[
= \begin{bmatrix} q_0^2 + q_1^2 + q_2^2 + q_3^2 & 0 & 0 \\ 0 & q_0^2 + q_1^2 + q_2^2 + q_3^2 & 2(q_1 q_2 - q_3 q_0) & 2(q_1 q_3 + q_2 q_0) \\ 0 & 2(q_1 q_2 + q_3 q_0) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(-q_1 q_0 + q_2 q_3) \\ 0 & 2(q_1 q_3 - q_2 q_0) & 2(q_1 q_0 + q_2 q_3) & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{bmatrix} p
\]

Finally, as we are interested in the imaginary part only of \(p' = (0, v')\), we suppress the first row and column and obtain the following linear transformation with a 3x3 rotation matrix:

\[
v' = \begin{bmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1 q_2 - q_3 q_0) & 2(q_1 q_3 + q_2 q_0) \\ 2(q_1 q_2 + q_3 q_0) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(-q_1 q_0 + q_2 q_3) \\ 2(q_1 q_3 - q_2 q_0) & 2(q_1 q_0 + q_2 q_3) & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{bmatrix} v
\]

\[
v' = [A(q)]v
\]

(27a)

(27b)

Note that the \([A(q)]\) matrix can be also expressed as a product between two matrices \([F(q)\mathbb{E}]\) and \([F(q)\mathbb{E}]\), obtained as submatrices of \([M(q)\mathbb{E}]\) e \([M(q^\ast)\mathbb{E}]\) in (26a):

\[
v' = \begin{bmatrix} +q_1 +q_0 -q_3 +q_2 \\ +q_2 +q_3 +q_0 -q_1 \\ +q_3 -q_2 +q_1 +q_0 \end{bmatrix} \begin{bmatrix} +q_1 +q_2 +q_3 \\ +q_0 -q_3 +q_2 \\ +q_3 +q_0 -q_1 \\ -q_2 +q_1 +q_0 \end{bmatrix} v
\]

\[
v' = [F(q)\mathbb{E}][F(q^\ast)]^T v
\]

(28a)

(28b)
where
\[
A(q) = [F(q)]_\oplus [F(q)]_\ominus^T
\]  
(29a)
\[
[F(q)]_\oplus = \begin{bmatrix} +q_1 & +q_0 & -q_3 & +q_2 \\ +q_2 & +q_3 & +q_0 & -q_1 \\ +q_3 & -q_2 & +q_1 & +q_0 \end{bmatrix}
\]  
(29b)
\[
[F(q)]_\ominus = \begin{bmatrix} +q_1 & +q_0 & +q_3 & -q_2 \\ +q_2 & -q_3 & +q_0 & +q_1 \\ +q_3 & +q_2 & -q_1 & +q_0 \end{bmatrix}
\]  
(29c)

**Algorithm 1:** Computes quaternion \( q \) given \([A] \) matrix

**Input:** matrix \([A]\)

**Output:** quaternion \( q \)

1. \( t_r = A_{0,0} + A_{1,1} + A_{2,2} \)
2. if \( t_r \geq 0 \)  
3. \( s = \sqrt{t_r + 1} \)  
4. \( q_0 = 0.5s \)  
5. \( q_1 = (A_{2,1} - A_{1,2})s \)  
6. \( q_2 = (A_{0,2} - A_{2,0})s \)  
7. \( q_3 = (A_{1,0} - A_{0,1})s \)  
8. else  
9. \( i = 0 \)  
10. if \( A_{1,1} > A_{0,0} \)  
11. \( i = 1 \)  
12. if \( A_{2,2} > A_{1,1} \) then \( i = 2 \)  
13. else \( i = 1 \)  
14. end  
15. if \( A_{2,2} > A_{0,0} \) then \( i = 2 \)  
16. if \( i == 0 \)  
17. \( s = \sqrt{A_{0,0} - A_{1,1} - A_{2,2} + 1} \)  
18. \( q_1 = 0.5s \)  
19. \( q_2 = (A_{0,1} + A_{1,0})s \)  
20. \( q_3 = (A_{2,0} + A_{0,2})s \)  
21. \( q_0 = (A_{1,2} - A_{2,1})s \)  
22. else  
23. \( i = 1 \)  
24. \( s = \sqrt{A_{1,1} - A_{2,2} - A_{0,0} + 1} \)  
25. \( q_2 = 0.5s \)  
26. \( s = 0.5s \)  
27. \( q_3 = (A_{1,2} + A_{2,1})s \)  
28. \( q_1 = (A_{0,1} + A_{1,0})s \)  
29. \( q_0 = (A_{0,2} - A_{2,0})s \)  
30. end  
31. if \( i == 2 \)  
32. \( s = \sqrt{A_{2,2} - A_{0,0} - A_{1,1} + 1} \)  
33. \( q_3 = 0.5s \)  
34. \( s = 0.5s \)  
35. \( q_1 = (A_{2,0} + A_{0,2})s \)  
36. \( q_2 = (A_{1,2} + A_{2,1})s \)  
37. \( q_0 = (A_{1,0} - A_{0,1})s \)  
38. return \( q \)

Just like it is possible to obtain a matrix of rotation \([A(q)]\) given a \( q \) quaternion, it is possible also to do viceversa: obtaining \( q \) given a 3x3 matrix \([A(q)]\). This is more complex, but still it does not presents problems of singularity. The transformation is expressed by Algorithm 1 that outputs \( q \) as a function of \([A]\).

Interesting: for a quaternion there is a single rotation matrix \([A(q)]\), viceversa given a \([A] \) matrix one can compute two quaternions, with opposite signs.
5. Rotation axis

It is known that one can express a finite rotation by providing an angle of rotation $\phi$ about an axis expressed as a unit-length vector $u$, and this is equivalent to the following unimodular quaternion:

\[ q_0 = \cos \left( \frac{\phi}{2} \right) \]
\[ q_1 = u_x \sin \left( \frac{\phi}{2} \right) \]
\[ q_2 = u_y \sin \left( \frac{\phi}{2} \right) \]
\[ q_3 = u_z \sin \left( \frac{\phi}{2} \right) \]

One can see that the norm of such quaternion is unitary for whatever value of $\phi$ and $u$, because of the property $\sin^2(\alpha) + \cos^2(\alpha) = 1$ and $|u| = 1$, in fact $|q|^2 = \cos^2(\phi/2) + (u_x^2 + u_y^2 + u_z^2)\sin^2(\phi/2) = 1$.

Among the many proofs that (23) expresses a rotation, for the interested reader here we report a geometric proof, inspired by Figure 1: remembering the property $\cos(\phi) = \cos^2(\phi/2) - \sin^2(\phi/2)$, $\sin(\phi) = 2\sin(\phi/2)\cos(\phi/2)$, $\cos(\phi)$ =
1 − 2 \sin^2(\phi/2), one has:

\[
p' = (0, v') = qpq^*
\]

\[
= \left(\cos \frac{\phi}{2}, u \sin \frac{\phi}{2}\right) \left(0, v\right) \left(\cos \frac{\phi}{2}, -u \sin \frac{\phi}{2}\right)
\]

\[
= \left(-\sin \frac{\phi}{2}(u \cdot v), \cos \frac{\phi}{2}v + \sin \frac{\phi}{2}(u \times v)\right) \left(\cos \frac{\phi}{2}, -u \sin \frac{\phi}{2}\right)
\]

\[
= \left(-\sin \frac{\phi}{2} \cos \frac{\phi}{2}(u \cdot v) + \sin \frac{\phi}{2} \cos \frac{\phi}{2}(v \cdot u) - \sin^2 \frac{\phi}{2}(u \times v) \cdot u, \\
\sin^2 \frac{\phi}{2}(u \cdot v) \cdot u + \cos^2 \frac{\phi}{2} v
\]

\[
+ \sin \frac{\phi}{2} \cos \frac{\phi}{2}(u \times u) - \sin \frac{\phi}{2} \cos \frac{\phi}{2}(v \times u) - \sin^2 \frac{\phi}{2}(u \times v) \times u\right)
\]

\[
= \left(0, \sin^2 \frac{\phi}{2}(u \cdot v) + \cos^2 \frac{\phi}{2} v + 2 \sin \frac{\phi}{2} \cos \frac{\phi}{2}(u \times v) - \sin^2 \frac{\phi}{2}(v - (u \cdot v)u)\right)
\]

\[
= \left(0, 2 \sin^2 \frac{\phi}{2}(u \cdot v) + \cos^2 \frac{\phi}{2} v - \sin^2 \frac{\phi}{2} v + 2 \sin \frac{\phi}{2} \cos \frac{\phi}{2}(u \times v)\right)
\]

\[
= \left(0, (1 - \cos \phi)(u \cdot v) + \cos \phi v + \sin \phi(u \times v)\right)
\]

\[
= \left(0, (u \cdot v)u + \cos \phi(v - (u \cdot v)u) + \sin \phi(u \times v)\right)
\]

The result, \(v' = (u \cdot v)u + \cos \phi(v - (u \cdot v)u) + \sin \phi(u \times v)\), matches the result that one could obtain by directly using Figure 1 and using vector operations (in figure, \(v_1 = (u \cdot v)u, v_2 = v - v_1\) and \(v_3 = u \times v_2 = u \times v\)).

It is also possible to do the inverse process, i.e. obtaining angle and axis of rotation given a quaternion, although one might incur into a singularity for \(\phi = 0 \pm n2\pi, n \in \mathbb{N}\):

\[
\phi = 2 \cos^{-1}(q_0) \tag{32a}
\]

\[
v = \begin{cases} q_1 \\ q_2 \\ \frac{1}{\sin \frac{\phi}{2}} \end{cases} \tag{32b}
\]

### 6. Angular velocity

One can use quaternion algebra also to compute velocity and acceleration of points belonging to coordinate system subject to angular velocity and angular acceleration.

By simple time derivative of \(0, v' = q(0,v)q^*\) it is possible to obtain absolute velocity \(\ddot{v}\) of the point. Using the notation \(\dot{q} = dq/dt\):

\[
p' = (0, v') = qpq^*
\]

\[
\dot{p}' = (0, \dot{v'}) = \frac{d(q \dot{p} q^*)}{dt}
\]

\[
\ddot{p}' = q \dot{p} q^* + q \dot{q} q^* + q \ddot{p} q^* \tag{33}
\]
as follows from the rule of derivative for the product of quaternions:

\[ d (q_a q_b) / dt = q_a \dot{q}_b + q_b \dot{q}_a \]

Sometimes (33) cannot be used directly because often one does not know \( \dot{q} \), but rather knows the angular velocity. So it is necessary to obtain a relation between \( \dot{q} \) and \( \omega \), the vector of angular velocity expressed in absolute reference or between \( \dot{q} \) and \( \omega_l \), the vector of angular velocity expressed in the local rotated reference.

To this end let consider \( \mathbf{v}' = [\mathbf{A}(q)] \mathbf{v} \), let perform the factorization (29a) and take the time derivative. Since it is generally \[ dv = [\dot{F}(q)_{\mathbb{E}}] \mathbf{v} + [F(q)_{\mathbb{E}}] \dot{\mathbf{v}} + [F(q)_{\mathbb{E}}] [\dot{F}(q)_{\mathbb{E}}]^T \dot{\mathbf{v}} \]

By performing the product between the two matrices, it is easy to show that in general \[ [F(q_{\mathbb{E}})]^T [F(q_{\mathbb{E}})] = [F(q_{\mathbb{E}})]^T [F(q_{\mathbb{E}})]^T \], hence (34) becomes:

\[ \mathbf{v}' = 2[F(q)_{\mathbb{E}}]^T \mathbf{v} + [F(q)_{\mathbb{E}}] [F(q)_{\mathbb{E}}]^T \mathbf{v} \]

At the same time it also holds:

\[ \mathbf{v}' = [\mathbf{A}(q)] \mathbf{v} \]
\[ \dot{\mathbf{v}}' = [A(q)] \mathbf{v} + [A(q)] \dot{\mathbf{v}} \]
\[ \ddot{\mathbf{v}}' = [A(q)] (\omega_l \times \mathbf{v}) + [A(q)] \ddot{\mathbf{v}} \]

where in (36b) we used \( \omega_l \), i.e., angular speed in the local rotated reference, as shown in many textbooks.

Equations (35) can be also compared to (36a) and (36b). From this comparison, remembering \[ [A(q)] = [F(q)_{\mathbb{E}}]^T [F(q)_{\mathbb{E}}] \] and \( \omega_l \times \mathbf{v} = [\omega_l] \mathbf{v} \), one obtains the following ways to express \([A(q)]\):

\[ [\dot{A}(q)] = 2[F(q)_{\mathbb{E}}]^T [F(q)_{\mathbb{E}}] \]
\[ = 2[F(q)_{\mathbb{E}}] [F(q)_{\mathbb{E}}]^T \]
\[ = [A(q)] [\omega_l] = [F(q)_{\mathbb{E}}]^T [\omega_l] \]
\[ = [\omega] [A(q)] = [\omega] [F(q)_{\mathbb{E}}]^T \]

Remember, in general \([\dot{A}(q)] \neq [A(\dot{q})]\).

To proceed further, we report the following properties, that hold only for unimodular quaternions, that is when \( q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1 \):

\[ [F(q)_{\mathbb{E}}]^T [F(q)_{\mathbb{E}}] = [F(q)_{\mathbb{E}}]^T [F(q)_{\mathbb{E}}] = [I] \]
\[ [F(q)_{\mathbb{E}}]^T [F(q)_{\mathbb{E}}] = [F(q)_{\mathbb{E}}] [F(q)_{\mathbb{E}}]^T = ([I] - q^* q^{\dagger \ast}) \]
Using (36b), (37b) and (37c) we obtain:

\[
[A(q)](\omega_t \times v) = [\dot{A}(q)]v \\
[A(q)][\dot{\omega_t}]v = [\dot{A}(q)]v \\
[\dot{\omega_t}] = [A(q)]^T[F(q)\otimes][\dot{F}(q)\otimes]^T
\] (39)

Substituting \([A(q)]^T = [F(q)\otimes][F(q)\otimes]^T\) in (39), because of (29a), then remembering (38b), one can write:

\[
[\dot{\omega}_t] = 2[F(q)\otimes][F(q)\otimes]^T[F(q)\otimes][\dot{F}(q)\otimes]^T \\
[\dot{\omega}_t] = 2[F(q)\otimes][(I - q^* q^*^T)][\dot{F}(q)\otimes]^T
\] (40)

Since \([F(q)\otimes]q = 0\), one can simplify (40):

\[
[\dot{\omega}_t] = 2[F(q)\otimes][\dot{F}(q)\otimes]^T
\] (41)

Simplifying the multiplications in (41) and remembering the definition of the hemi-symmetric matrix \([\dot{\omega}_t]\), one can finally obtain \(\omega_t\) as a function of the derivative of quaternion \(\dot{q}\), in the following equivalent ways:

\[
\omega_t = -2[F(q)\otimes]\dot{q}^* = +2[F(q^*)\otimes]\dot{q} \quad (42a) \\
= +2[F(\dot{q})\otimes]\dot{q}^* = -2[F(q^*\otimes)\dot{q}] \quad (42b)
\]

At the same time one can express \(\omega_o\), angular velocity in absolute reference, remembering that \(\omega_t = [A(q)]^T\omega_o\):

\[
\omega_o = -2[F(q)\otimes]\dot{q}^* = +2[F(q^*)\otimes]\dot{q} \quad (43a) \\
= +2[F(\dot{q})\otimes]\dot{q}^* = -2[F(q^*\otimes)\dot{q}] \quad (43b)
\]

As an alternative to matrix expressions (42a), (42b), (43a), (43b), it is possible to obtain \(\omega_t\) and \(\omega_o\) using only the quaternion algebra. Introducing the following pure quaternions: \(q_{\omega_t} = (0, \omega_t) q_{\omega_o} = (0, \omega_o)\), with \(q_{\omega_t}, q_{\omega_o} \in \text{Im}\mathbb{H}\). Let compare \(\dot{v}' = \omega_o \times v_o + [A]\dot{v}\) with (33), and recall that for (25) one has \(p = q_s p' q_s^*\):

\[
\dot{q} p q^* + q p \dot{q}^* = (0, \omega_o \times v_o) \\
\dot{q} q^* p' q q^* + q q^* p' q \dot{q}^* = (0, \omega_o \times v_o)
\]

By making use of the property \(q q^* = 1\) and of the time derivative of such property \(\dot{q} q^* + \dot{q}^* q = 0\), one gets the simplified expression:

\[
\dot{q} q^* p' - p' q \dot{q}^* = (0, \omega_o \times v_o) \quad (44)
\]

Also, given the multiplicative properties (17b), the pure quaternion \((0, \omega_o \times v_o)\) can be expressed in the form \(\frac{1}{2}[(0, \omega_o)p' - p'(0, \omega_o)]\), obtaining:

\[
\dot{q} q^* p' - p' q \dot{q}^* = \frac{1}{2}[(0, \omega_o)p' - p'(0, \omega_o)]
\]
From this relation one obtains\textsuperscript{2}

\[(0, \omega_o) = 2 \dot{q} q^* \]  

(45)

Since for unimodular quaternions \(q^{-1} = q^*\), one also gets the inverse relation:

\[\dot{q} = \frac{1}{2} (0, \omega_o) q \]  

(46)

Equally useful as (45) and (46) are the analogous relations that use angular velocities in the local reference \(\omega_l\), substituting \((0, \omega_o) = q (0, \omega_l) q^*\) in (46) and simplifying:

\[(0, \omega_l) = 2 q^* \dot{q} \]  

(47a)

\[\dot{q} = \frac{1}{2} q (0, \omega_l) \]  

(47b)

As an alternative, by using matrix algebra and remembering (20), (29b) and (29c), one can express (46) and (47b) as:

\[\dot{q} = \frac{1}{2} [F(q^*)] T \omega_o \]  

(48a)

\[\dot{q} = \frac{1}{2} [F(q^*)] T \omega_l \]  

(48b)

### 7. Angular acceleration

By performing a second time derivative, one can get the relation between the angular acceleration \(\alpha = \dot{\omega}\) and the quaternion double derivative \(\ddot{q}\).

In detail lets introduce the pure quaternion \(q_{\alpha_l} = (0, \alpha_l)\) to express the angular acceleration in local coordinates, and \(q_{\alpha_o} = (0, \alpha_o)\) for the angular acceleration in absolute coordinates. By taking the derivative in (46) and (47b), one obtains the two equivalent expressions:

\[\ddot{q} = \frac{1}{2} (0, \alpha_o) q + \frac{1}{2} (0, \omega_o) \dot{q} \]  

(49a)

\[\ddot{q} = \frac{1}{2} \dot{q} (0, \omega_l) + \frac{1}{2} q (0, \alpha_l) \]  

(49b)

It is possible to obtain the inverse relations too, to get \(\alpha_l\) or \(\alpha_o\) given the quaternion \(\ddot{q}\). To this end lets take the time derivative of (45) and (47a):

\[(0, \alpha_o) = 2 \dot{q} q^* + 2 \dot{\dot{q}} \dot{q}^* \]  

(50a)

\[(0, \alpha_l) = 2 \dot{q}^* \dot{q} + 2 q^* \ddot{q} \]  

(50b)

\textsuperscript{2}Equation (44) provides only the imaginary part of \((0, \omega_o)\); but it would hold also for a generic \((a, \omega_o)\), with whatver \(a\). The fact that \(a\) follows from the fact that, given \(|q| = 1\), one gets \(q_0 q_0 + \dot{q}_1 q_1 + \dot{q}_2 q_2 + \dot{q}_3 q_3 = 0\). It follows that the real part of \(q q^*\) or \(q^* \dot{q}\) is null.
Of course one can express the same relations by using the matrix algebra, for instance performing the derivative of (42a) and (43a):

$$\alpha_l = -2[F(q)\odot]q^* - 2[F(q)\odot]\dot{q}^*$$ (51a)

$$\alpha_o = -2[F(q)\odot]q^* - 2[F(q)\odot]\dot{q}^*$$ (51b)

Note that the computation of the $2[F(q)\odot]\dot{q}^*$ and $2[F(q)\odot]\dot{q}^*$ terms is superfluous as they are always null (this can be verified by remembering that $q_0\dot{q}_0 + q_1\dot{q}_1 + q_2\dot{q}_2 + q_3\dot{q}_3 = 0$, as follows by taking the time derivative of the constraint over the unit norm: $qq^* = 1$).

Moreover, by taking the time derivative of (48a) and (48b), one obtains also:

$$\ddot{q} = \frac{1}{2}[F(q^*)\odot]^T\omega + \frac{1}{2}[F(q^*)\odot]^T\alpha_o$$ (52a)

$$\ddot{q} = \frac{1}{2}[F(q^*)\odot]^T\omega + \frac{1}{2}[F(q^*)\odot]^T\alpha_l$$ (52b)

Note that the acceleration of a point given $\dot{q}$ and $\ddot{q}$ can be derived directly by taking the time derivative of (33):

$$\dddot{q} = \ddot{q}p + \dot{q}p\dot{q}^* + \dot{q}p\dot{q}^* + \dot{q}\dot{p}\dot{q}^* + \dot{q}\dot{p}\dot{q}^* + \dot{q\dot{q}^*} + \dot{q}\dot{p}\dot{q}^* + \dot{q\dot{q}^*} + \dot{q}\dot{p}\dot{q}^* + \dot{q}\dot{p}\dot{q}^* + \dot{q}\dot{p}\dot{q}^*$$

$$= \ddot{q}p + \dot{q}p\dot{q}^* + \dot{q}p\dot{q}^* + 2\dot{q}p\dot{q}^* + 2\dot{q}\dot{p}\dot{q}^* + 2q\dot{p}\dot{q}^* + 2q\dot{p}\dot{q}^*$$ (53)

The results obtained herein are summed up in the following table (2), for a rapid and concise reference.

### 8. Lie groups, exponentials and relation with other representations

Rotations in 3D can be approached with the tools of Lie groups and Lie algebras. The following is a list of useful concepts in Lie groups in the context of rotations.

- A **Lie group** is a group $G$ that is also a differentiable manifold. As a group it is an algebraic structure with properties of closure, associativity, presence of identity element and inverse element for product between its elements. Examples:

  - $\mathbb{R}^n$, the Euclidean space with addition,
  - $\text{GL}(n, \mathbb{R})$, the general linear group of invertible nxn matrices and their product,
  - $\text{SL}(n, \mathbb{R})$, the special linear group of matrices with det = 1,
  - $\text{SO}(n)$, the special orthogonal group of orthogonal matrices with det = 1,
  - $\text{SU}(n)$, the special unitary group of complex matrices with det = 1,
Table 2: Main relations for angular acceleration and angular velocity, and quaternions

- $\mathbb{H}_1$, the group of unit-length quaternions, also compact symplectic group $Sp(1)$,
- $Spin(n)$, the spin group.

For kinematics and dynamics, the SO(3) special orthogonal group is important as it deals with rotation matrices in 3D space.

- For rotations in 2D, a rotation $\alpha$ can be expressed by a unit-length complex number $e^{i\alpha}$ in the $C_1$ group, also $U(1)$, and $Spin(2)$. Topologically this is the circle $S^1$. All them are isomorphic to $SO(2)$.
- For rotations in 3D, $\mathbb{H}_1$, SU(2) and Spin(3) are all isomorphic, and simply connected. All them are topologically the $S^3$ sphere. All them are double covers of $SO(3)$, which is double connected. A practical consequence: two opposite quaternions $-\rho$ and $+\rho \in \mathbb{H}_1$ represent the same single rotation matrix $R \in SO(3)$.
- A Lie algebra is a vector space $\mathfrak{g}$ equipped with a non-associative alternating bilinear map $\mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$; $(x, y) \mapsto [x, y]$, named Lie bracket.
- Given a Lie group $G$, the tangent bundle at the identity $T_1G$, together with a Lie bracket, forms the Lie algebra $\mathfrak{g}$ of the Lie group $G$. Examples:
  - the Lie algebra of $U(1)$ is $\mathfrak{u}(n)$, isomorphic to $\mathbb{R}$;
the Lie algebra of $SO(n)$ is $\mathfrak{so}(n)$, the algebra of skew-symmetric $n \times n$ real matrices,

- the Lie algebra of $\mathbb{H}_1$ is $\text{Im}(\mathbb{H})$, the algebra of pure quaternions (quaternions with no real part),

- in particular, the Lie algebras of $SO(3)$, $SU(3)$, $\text{Spin}(3)$ and $\mathbb{H}_1$ are all isomorphic to the Lie algebra $\mathfrak{so}(3)$, the algebra of skew symmetric $3 \times 3$ matrices $\tilde{a}$ such that $\tilde{a}b = a \times b$.

- Let $\gamma : \mathbb{R} \to G$ be a one parameter sub-group of $G$, i.e. for which $\gamma(0) = I$, the identity element in $G$. The exponential map $\exp : \mathfrak{g} \to G$ is defined as $\exp(\omega) = \gamma(1)$, for $\omega \in \mathfrak{g}$. One can see that $\exp(t\omega) = \gamma(t)$, and that $\dot{\gamma}(0) = \omega$. In practical terms, the exponential map connects elements in Lie algebras to underlying Lie groups.

- For an element $R$ in Lie group $SO(3)$ and an element $\delta \Theta$ in the corresponding Lie algebra $\mathfrak{so}(3)$, one has

\[
R = \exp(\delta \Theta) \quad (54)
\]
\[
\delta \Theta = \log(R) \quad (55)
\]

- One can extract the three dimensional rotation pseudovector $\delta \theta$ from $\delta \Theta$ and vice versa, via

\[
\delta \Theta = \text{axis}(\delta \Theta) \quad (56)
\]
\[
\delta \Theta = \text{skew}(\delta \theta) = \hat{\delta \theta} \quad (57)
\]

For our purposes, $\delta \theta$ can be considered a (not necessarily infinitesimal) incremental rotation; for example in a time stepper one could have $\delta \theta = \omega dt$.

- Just like in (54) and (55), an exponential map links $\mathbb{H}_1$, (unit quaternions), and its Lie algebra $\text{Im}(\mathbb{H})$ of pure quaternions $\delta \rho = [0, \delta v]$:

\[
\rho = \exp(\delta \rho) \quad (58)
\]
\[
\delta \rho = \log(\rho) \quad (59)
\]

- The exponential map (58) can be explicitly computed using the closed-form expression $\exp([s, v]) = e^s \left[ \cos(||v||), \frac{v}{||v||} \sin(||v||) \right]$, hence:

\[
\exp([0, \delta v]) = \left[ \cos(||\delta v||), \frac{\delta v}{||\delta v||} \sin(||\delta v||) \right] \quad (60)
\]
\[
\exp([0, u \beta]) = [\cos(\beta), u \sin(\beta)] \quad \text{for } ||u|| = 1 \quad (61)
\]

- We can use the pure and imag operators to convert pure quaternions $[0, \delta v]$ from and to rotation pseudovectors $\delta \theta$ by observing that $\delta v = \frac{1}{2} \delta \theta$:

\[
\delta \theta = 2 \text{imag}(\delta \rho) \quad (62)
\]
\[
\delta \rho = \frac{1}{2} \text{pure}(\delta \theta) \quad (63)
\]
More succinctly, we can introduce the \textit{axis} and \textit{qskew} operators:

\begin{align}
\delta \theta &= \text{axis}(\delta \rho) \\
\delta \rho &= \text{qskew}(\delta \theta)
\end{align}

\begin{align}
\delta \theta &= \text{axis}(\delta \rho) = \text{axis}(\log(\rho)) = 2v \frac{||v||}{||v||} \tan^{-1}\left(\frac{||v||}{s}\right)
\end{align}

Note that the last expression is singular for zero rotations, so when $||v|| < \epsilon$ one can compute it as the simplified expression $\delta \theta = 2v$, also note that rather than using $\tan^{-1}(\cdot)$ it is advisable to use atan2().

Functions (66) and (67) are available in the \texttt{chrono::ChQuaternion} class as \texttt{Q.to_Rotv} and \texttt{Q.from_Rotv}, respectively.

The scalar exponential of a quaternion is

\begin{align}
q^t &= [\cos(\beta), u \sin(\beta)]^t \\
&= \exp([0, u \beta])^t \\
&= \exp([0, u \beta]) \\
q^t &= [\cos(\beta t), u \sin(\beta t)]
\end{align}

\section{Other properties}

\subsection{Normalization of quaternions}

Only unimodular quaternions $|q_n| = 1$ can be used for expressing rotations, $q \in S^3$. Sometimes, however, it might happen that numerical roundoff errors, or approximations in time integration schemes, or other sources of numerical errors, will gradually introduce a drift on quaternions, that gradually depart from the unit hypersphere. Hence it may be necessary to periodically check that quaternions really have unit norm, and if not, they should be normalized using a formula that exploits the (13c) property:

\begin{align}
q_n = q \frac{1}{||q||}
\end{align}

\subsection{Interpolating quaternions}

Interpolating finite rotations in 3D space is not trivial. One cannot just do a linear interpolation of $q_a$ and $q_b$ with a formula like $q(t) = (1-t)q_a + tq_b$,
because it does not guarantee that \( q(t) \in S^3 \). A custom interpolation that preserves the unit length of \( q(t) \) must be used.

By leveraging on these properties, one can solve the interpolation by performing:

\[
q_b = q_a q_a^{-1} q_b q_a^{-1} \quad \text{or} \quad (q_b q_a^{-1}) (q_a p q_a^{-1}) q_b^{-1} = q_b (q_a p q_a^{-1}) q_b^{-1}
\]

where \( q_\Delta = q_a q_b^{-1} \), unimodular quaternion because of (13e), represents the rotation from \( q_a \) to \( q_b \). Representing \( q_\Delta = (\cos(\theta_\Delta), u_\Delta \sin(\theta_\Delta)) \), one sees that \( q_\Delta \) operates a rotation of an angle \( 2\theta_\Delta \) about the fixed axis \( u_\Delta \). By parametrizing such rotation as a function of the angle \( \theta \) increasing with time \( t \) one will get \( q_\delta(t) = (\cos(\theta_\Delta t), u_\Delta \sin(\theta_\Delta t)) \).

Recalling (68) (power of a quaternion \( q \in S^3 \), one gets:

\[
q_\delta(t) = (\cos(\theta_\Delta t), u_\Delta \sin(\theta_\Delta t))
\]

\[
= (\cos(\theta_\Delta t), u_\Delta \sin(\theta_\Delta t))^t
\]

\[
= q_\Delta
\]

\[
= (q_b q_a^{-1})^t
\]

That is, recalling (70a), the \( \rho_{(q_a, q_b)}(t) \) quaternion that interpolates \( q_a \) and \( q_b \), assuming initial value \( \rho_{(q_a, q_b)}(0) = q_a \) and final value \( \rho_{(q_a, q_b)}(1) = q_b \), is given by the formula \( q_b q_a^{-1} \), that is:

\[
\rho_{(q_a, q_b)}(t) = (q_b q_a^{-1})^t q_a
\]

By the way:

\[
\rho_{(q_a, q_b)}(t) = (-\theta_\Delta \sin(\theta_\Delta t), \theta_\Delta u_\Delta \cos(\theta_\Delta t)) q_a
\]

\[
|\rho_{(q_a, q_b)}(t)| = |\theta_\Delta| 1 = |\theta_\Delta|
\]

From a computational outlook, rather than getting \( \rho_{(q_a, q_b)}(t) \) from (72), it is better to perform the following steps: \( q_\Delta = q_b q_b^{-1} \), then evaluate \( \theta_\Delta = \cos^{-1}(q_\Delta) \) and \( u_\Delta = \{q_{\Delta 1}, q_{\Delta 2}, q_{\Delta 3}\}^T 1/|\sin(\theta_\Delta)| \), and finally compute \( q_\delta(t) = (\cos(\theta_\Delta t), u_\Delta \sin(\theta_\Delta t)) \) and get \( \rho_{(q_a, q_b)}(t) = (\cos(\theta_\Delta t), u_\Delta \sin(\theta_\Delta t)) q_a \).

This (spherical, linear) interpolation is often called SLERP. As an alternative formulation of SLERP, recalling (72) and using trigonometric properties:

\[
\rho_{(q_a, q_b)}(t) = q_a \frac{\sin[\theta_\Delta (1 - t)]}{\sin \theta_\Delta} + q_b \frac{\sin(\theta_\Delta t)}{\sin \theta_\Delta}
\]

In all cases there is a singularity for \( q_a = \pm q_b \).
### 9.3 Other interpolation types

In **Chrono::Engine** we implemented the SLERP and other rotation interpolation methods as subclasses of the **chrono::ChFunctionRotation** class. In detail,

- **chrono::ChFunctionRotation_ABCfunctions** uses three functions for three angles (Euler angles, Cardano angles, etc., btw there are various non equivalent angle sequences) so that $\rho(t) = \rho(R(t))$ where the rotation matrix is a concatenation of three rotations $R(t) = R_C(t)R_B(t)R_A(t)$.

- **chrono::ChFunctionRotation_axis** takes a fixed rotation axis $v$ and a function $\alpha = f_\alpha(t)$ to build the rotation $\rho(t) = \rho(v, f_\alpha(t))$.

- **chrono::ChFunctionRotation_setpoint** computes the quaternion and its derivatives from a continuously updated setpoint passed from an external sampled function.

- **chrono::ChFunctionRotation_spline** computes the quaternion using quaternion B-Splines, of order $p$, given $N$ quaternion control points: $\rho(t) = \rho(\rho_1, \rho_2, ..., \rho_N, t)$ . The first and last rotation are matched exactly, whereas the intermediate control points are passed nearby, just like in usual B-splines. Note that the SLERP interpolation described in previous section is obtained exactly with this method, when using order $p = 1$ (linear spline).

- **chrono::ChFunctionRotation_SQUAD** computes the quaternion using a sequence of SQUAD interpolations, given $N$ quaternion control points: $\rho(t) = \rho(\rho_1, \rho_2, ..., \rho_N, t)$ . All control point rotations are matched exactly, because the class takes the sequence of control points, and for each span it inserts two ghost rotations so that each span is like a single SQUAD as in classic literature.

### 10. Conclusion

Quaternions are extensively used in **Chrono::Engine** to work with rotations. Look into the documentation of the the **chrono::ChQuaternion** class for additional information.

More information available in **Chrono::Engine** web site.

### References
