The Quaternions with an application to Rigid Body Dynamics

Evangelos A. Coutsias† and Louis Romero‡
Department of Mathematics and Statistics,
University of New Mexico
Albuquerque, NM 87131

Friday 12 February 1999

1 Brief History

William Rowan Hamilton invented the quaternions in 1843, in his effort to construct *hypercomplex* numbers, or higher dimensional generalizations of the complex numbers. Failing to construct a generalization in three dimensions (involving "triplets") in such a way that division would be possible, he considered systems with four complex units and arrived at the **quaternions**. He realized that, just as multiplication by i is a rotation by 90^o in the complex plane, each one of his complex units could also be associated with a rotation in space. Vectors were introduced by Hamilton for the first time as "pure quaternions" and Vector Calculus was at first developed as part of this theory. Maxwell's Electromagnetism was first written using quaternions (see, eg. [6]).

2 Basic Notation and Definitions

We will define a quaternion using a scalar and a three dimensional vector. We can write the quaternion q as

$$q = (a, \underline{b})$$

We could also use the notation

$$q = a + \underline{b},$$

or

$$q = ae_0 + b_1e_1 + b_2e_2 + b_3e_3\ ,$$

with the latter being the most explicit, exhibiting the space of quaternions, $\mathcal{Q}$, as a four dimensional vector space over the real numbers with basis elements e_0, e_1, e_2, e_3. However, in these notes we prefer the first of these notations.

Given two quaternions $q_1 = (a_1, \underline{b_1})$, and $q_2 = (a_2, \underline{b_2})$ we can define the addition and multiplication of quaternions.

Definition 1 *The addition of two quaternions is defined as*

$$q_1 + q_2 = (a_1 + a_2, \underline{b}_1 + \underline{b}_2)$$

Definition 2 *The multiplication of two quaternions is defined as*

$$q_1 q_2 = (a_1 a_2 - \underline{b}_1 \cdot \underline{b}_2, a_1 \underline{b}_2 + a_2 \underline{b}_1 + \underline{b}_1 \times \underline{b}_2)$$

Here $\underline{b}_1 \cdot \underline{b}_2$ *is the dot product, and* $\underline{b}_1 \times \underline{b}_2$ *is the cross product of the two vectors.*

We also use the following definition.

Definition 3 *The conjugate of a quaternion* $q = (a, \underline{b})$ *is defined as*

$$q^c = (a, -\underline{b})$$

It is straightforward to verify all of the following properties.

- The quaternion $e_0 = (1, 0)$ is the multiplicative identity. That is, for any quaternion q we have $e_0 q = q e_0 = q$. Furthermore, multiples of e_0 commute with any quaternion q and they are the only quaternions with that property. That is $(a, 0)q = q(a, 0)$.
- For the other basis elements, e_1 , $i = 1, 2, 3$, the rules of multiplication are $e_l e_k = \epsilon_{lkj} e_j - \delta_{lk} e_0$, $l, k = 1, 2, 3$.
- The product $q^c q = (a^2 + \underline{b} \cdot \underline{b}, 0)$ can be thought of as the norm of the quaternion. We define
$$N(q) := q q^c.$$
- The norm is multiplicative:
$$N(q_1 q_2) = N(q_1) N(q_2).$$
- For any quaternion $q = (a, \underline{b})$ that is not identically zero, we have
$$q^{-1} = \frac{(a, -\underline{b})}{q q^c}.$$
That is, $q^{-1} q = q q^{-1} = e$. This establishes $\mathcal{Q} \setminus \{0\}$ as a *Division Algebra.*
- The set of quaternions of unit norm,
$$\mathcal{Q}_1 := \{q | N(q) = 1\} \ ,$$
forms a subgroup of $\mathcal{Q} \setminus 0$, while the set of pure quaternions
$$\mathcal{Q}_0 := \{q | q = (0, \underline{v})\} \ ,$$
is a 3-dimensional vector space over the reals, which we identify with $\mathbf{R}^3$.

- In general the multiplication of two quaternions is not a commutative operation. That is, $q_1 q_2 \neq q_2 q_1$. In particular, division by $q \neq 0$ must be defined as left or right multiplication by q^{-1}, giving in general different results. However, the additon of quaternions is commutative.
- The associative law holds for multiplication and addition.
- The distributive law holds.

Of these properties the associative law for multiplication is probably the least obvious, but can easily be verified by direct computation. These properties can be summarized in the following theorem.

Theorem 1 *Using our definition of addition and multiplication, the quaternions form a noncommutative field.*

3 Reflections

In what follows we will need to use the vector identity

$$(\underline{a} \times \underline{b}) \times \underline{c} = \underline{b}(\underline{a} \cdot \underline{c}) - \underline{a}(\underline{b} \cdot \underline{c})$$

Suppose we associate the pure quaternions $v = (0, \underline{v})$ with the vector $\underline{v}$, and $n = (0, \underline{n})$ with the vector $\underline{n}$. If we define the operation

$$v' = nvn,$$

an explicit calculation shows that

$$v' = (0, \underline{v}')$$

where

$$\underline{v}' = (\underline{n} \times \underline{v}) \times \underline{n} - \underline{n}(\underline{n} \cdot \underline{v})$$

Using our identity for the cross product this can be written as

$$\underline{v}' = \underline{v} - 2\underline{n}(\underline{n} \cdot \underline{v})$$

If $\underline{n}$ is a unit vector, the vector $\underline{v}'$ is the reflection of $\underline{v}$ in the plane normal to $\underline{n}$.

We summarize this in a theorem.

Theorem 2 *If $v = (0, \underline{v})$, and $n = (0, \underline{n})$, where $\underline{n}$ is a unit vector, then $nvn = v' = (0, \underline{v}')$ where $\underline{v}'$ is the vector obtained by reflecting $\underline{v}$ about the plane perpendicular to $\underline{n}$ (and passing through the origin).*

4 Rotations as the Product of Reflections

In order to understand how to represent rotations using quaternions it is helpful to understand a theorem concerning the representation of a rotation as the product of two reflections. This theorem is very simple in two dimensions. Suppose we perform a reflection S_1 about a line l_1, followed by a reflection S_2 about a line l_2. The combination of these two operations $R = S_2S_1$ clearly leaves the point of intersection Q of the two lines fixed. The operation is a proper isometry (distance and orientation preserving transformation) that leaves the point Q fixed. It follows that the operation is a rotation about the point Q. It only remains to find what the angle of the rotation is. In order to do this we draw the picture: the reflection S_1 leaves the line l_1 invariant. The reflection S_2 reflects the line l_1 into the line l_1'. Clearly the angle between the lines l_1 and L_1' is 2θ if θ is the angle between the lines l_1 and l_2. The proves the following theorem.

Theorem 3 *If we perform a reflection S_1 about a line l_1 followed by a reflection S_2 about the line l_2, the resulting transformation is a rotation about the point of intersection Q of the two lines. The rotation is from the line l_1 to the line l_2, and by an angle 2θ, where θ is the angle between the two lines.*

This construction clearly holds for three dimensional rotations (Figure 1). In order to rotate by θ about a line l we need to reflect about two planes that are at an angle $\theta/2$, and that intersect at the line l. Suppose the line l passes through the origin, and in the direction $\underline{p}$ where $\underline{p}$ is a unit vector. In this case we need to choose our two planes so they also pass through the origin. If the normals to the two planes are given by $\underline{n}_1$ and $\underline{n}_2$, then we can combine the two reflections to get a rotation about the line in the direction $\underline{p}$ provided $\underline{n}_2 \times \underline{n}_1 = sin(\theta/2)\underline{p}$, and $\underline{n}_1 \cdot \underline{n}_2 = cos(\theta/2)$.

Theorem 4 *Let $\underline{p}$, $\underline{n}_1$ and $\underline{n}_2$ be unit vectors. Let S_i be the reflection about a plane passing through the origin, and normal to $\underline{n}_i$. If $\underline{n}_2 \times \underline{n}_1$ is in the direction $\underline{p}$, then S_2S_1 is a rotation about the line in the direction $\underline{p}$. If the angle between the vectors $\underline{n}_1$ and $\underline{n}_2$ is $\theta/2$, then the rotation is by an angle of θ. In this case we have $\underline{n}_1 \cdot \underline{n}_2 = cos(\theta/2)$, and $\underline{n}_2 \times \underline{n}_1 = sin(\theta/2)\underline{p}$*

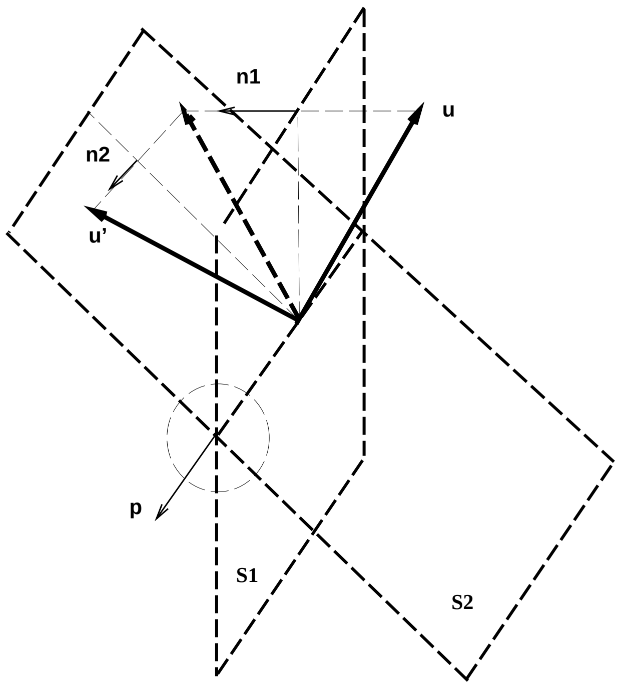

Figure 1. Rotation as two successive reflections

5 The Representation of Rotations Using Quaternions

Suppose we want to rotate by θ about a line passing through the origin, and pointing in the direction $\underline{p}$. The theorem in the last section shows that we can accomplish this by performing the reflections S_2S_1 of the last theorem. In terms of quaternions this transformation maps the vector $\underline{v}$ to the vector

$$v' = n_2n_1vn_1n_2$$

We can write this as

$$v' = C_q(v) := qvq^{-1}$$

where

$$q = n_2n_1 \ .$$

In order to do this we have used the fact that since n_i is associated with a unit vector, then $n_i^{-1} = -n_i$, and also the fact that $(n_2n_1)^{-1} = n_1^{-1}n_2^{-1}$. A direct calculation shows that

$$q = \pm(cos(\theta/2), sin(\theta/2)\underline{p})$$

where $\underline{p}$ is a unit vector and the sign depends on the choice of unit normals for the two planes (the choice shown in Fig. 1 corresponds to the (-) sign). Clearly, the rotation is independent of the sign of q. This proves the following theorem:

Theorem 5 *Let $q = (cos(\theta/2), sin(\theta/2)\underline{p})$ where $\underline{p}$ is a unit vector. Let $v = (0, \underline{v})$. The transformation qvq^{-1} maps v into $v' = (0, \underline{v}')$, where $\underline{v}'$ is obtained by rotating $\underline{v}$ about the $\underline{p}$ axis by θ.*

We examine now the mapping $q \to C_q$ of the division algebra $\mathcal{Q} \setminus \{0\}$ into the group of linear transformations of $\mathcal{Q}$ into itself. It is easy to see that it is a homomorphism, since

$$C_q(C_p(u)) = q(pvp^{-1})q^{-1} = (qp)v(qp)^{-1} = C_{qp}(v).$$

Moreover,

$$C_q(uv) = q(uv)q^{-1} = (quq^{-1})(qvq^{-1}) = C_q(u)C_q(v) \ .$$

We call the action of C_q on an element v a *conjugation* of v by $q \neq 0$. Conjugations have the following properties:

- C_q is norm-preserving:

$$N(C_q(v)) = N(q)N(v)N(q^{-1}) = N(v) \ .$$

- All possible conjugations can be found by considering $q \in \mathcal{Q}_1$. Indeed, if $q = \alpha p$, with $\alpha \neq 0$ scalar, then $C_q = C_p$.

- $C_q = C_{-q}$.

For the purpose of studying rotations in $\mathbf{R}^3$, we restrict our attention to C_q acting on v with $q \in \mathcal{Q}_1$, $v \in \mathcal{Q}_0 \equiv \mathbf{R}^3$. Then it is easy to see that $v' = C_q(v) \in \mathbf{R}^3$:

$$(v')^c = (C_q(v))^c = (qvq^c)^c = qv^cq^c = -qvq^c = -v' \ ,$$

where we recall that $v \in \mathcal{Q}_0$ if and only if $v^c = -v$ and for $q \in \mathcal{Q}_1$ we have $q^{-1} = q^c$. We also recall that $q, p \in \mathcal{Q}_1$ implies that $qp \in \mathcal{Q}_1$.

Orientation in $\mathbf{R}^3$ is defined, as usual, by the triple scalar product. Thus, the three vectors $\underline{a}$, $\underline{b}$, $\underline{c}$ form a *right-handed system* if $\text{sign}(\underline{a} \cdot (\underline{b} \times \underline{c})) = +1$. The dot product of two pure quaternions u, v can be defined naturally as the scalar

$$u \cdot v = (\underline{u} \cdot \underline{v}, 0) = -\frac{uv + vu}{2} \ ,$$

while their cross-product can be defined as the pure quaternion

$$u \times v = (0, \underline{u} \times \underline{v}) = \frac{uv - vu}{2} \ .$$

Since conjugation respects multiplication of quaternions, it also respects the dot and cross products in $\mathcal{Q}_0$. Thus

$$C(u \cdot (v \times w)) = C_q(u) \cdot (C_q(v) \times C_q(w)) \ .$$

Since conjugation leaves scalars invariant, $C(u \cdot (v \times w)) = u \cdot (v \times w)$ and orientation is clearly preserved by conjugation. Thus, conjugation is a linear, orientation preserving isometry of $\mathcal{Q}_0 \equiv \mathbf{R}^3$ onto itself, i.e. a proper orthogonal transformation. That all such transformations can be thus obtained follows from theorem 5. Now we see that C_q is a $2 \to 1$ group homomorphism of the $\mathcal{Q}_1$ onto $SO(3, \mathbf{R})$, with $\pm q \in \mathcal{Q}_1$ giving the same orthogonal transformation. Of course, this correspondence was established explicitly in theorem 5. Now we see how rotations can be composed:

Theorem 6 *The composition of two successive rotations, about axes $\underline{p}_1$ and $\underline{p}_2$, and by angles θ_1 and θ_2, respectively, results in a rotation about axis $\underline{p}_3$ by angle θ_3 given in terms of the quaternion $q_3 = q_2 q_1$ where*

$$q_i = \Big(\cos(\theta_i/2), \sin(\theta_i/2)\underline{p}_i\Big) \ , \ i = 1, 2, 3 \ .$$

Example: Consider the regular octahedron with vertices at $A = (+1, 0, 0)$, $B = (-1, 0, 0)$, $C = (0, +1, 0)$, $D = (0, -1, 0)$, $E = (0, 0, +1)$ and $F = (0, 0, -1)$. Clearly, a rotation by $\pi/2$ about the x-axis maps the octahedron into itself. Followed by a rotation by $\pi/2$ about the y-axis (which also maps the octahedron into itself), the net effect is to map the vertices as follows: $A \to (0, 0, -1)$, $B \to (0, 0, +1)$, $C \to ((+1, 0, 0)$, $D \to (-1, 0, 0)$, $E \to (0, -1, 0)$ and $F \to (0, +1, 0)$. Thus, the face AFC has rotated into itself by $2\pi/3$ about its outward normal ($AFC \to CAF$) and the face EDB has rotated into itself by $-2\pi/3$ about its own outward normal $EDB \to BED$). In terms of quaternions:

$$(\cos(\pi/4), \sin(\pi/4)\underline{j})(\cos(\pi/4), \sin(\pi/4)\underline{i}) = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\frac{\underline{i} + \underline{j} + \underline{j} \times \underline{i}}{\sqrt{3}}\right)$$

so that the net rotation is about the axis $(\underline{i} + \underline{j} - \underline{k})/\sqrt{3}$ by angle $2\pi/3$.

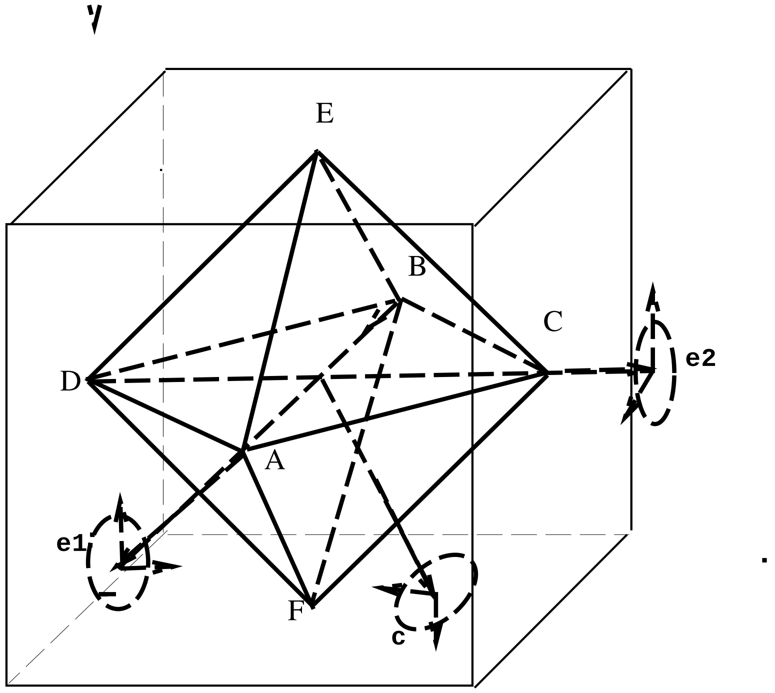

Figure 2. Rotating the octahedron: a rotation by 90^o about the x-axis, followed by a rotation by 90^o about the y-axis, produces a net rotation of 120^o about **c**, the normal from the origin to the face AFC.

6 Representation of unit quaternions as 3X3 orthogonal matrices.

We recall some facts about rotation matrices in 3-space; in the following discussion $Q \in \mathbf{R}^3$ will be an orthogonal matrix.

- The defining property of an orthogonal matrix is:

$$QQ^T = I.$$

- If $\underline{x}$ is an eigenvector, we have:

$$Q\underline{x} = \lambda\underline{x} \Rightarrow Q\underline{x}^\star = \lambda^\star \underline{x}^\star$$

so that

$$(\underline{x}^\star)^T \underline{x}^\star = (\underline{x}^\star)^T Q^T Q \underline{x}^\star = (\underline{x}^\star)^T \lambda^\star \lambda \underline{x}^\star \ .$$

so that $\lambda^\star\lambda = 1$. Since the characteristic polynomial is a real cubic, one of the roots must be real. Restricting to $Q \in SO(3, \mathbf{R})$ (i.e. $detQ = 1$), the roots must be 1, $e^{i\phi}$ and $e^{-i\phi}$. Thus

$$TrQ = 1 + 2\cos\phi$$

.

- The eigenvector $\underline{x}$ of eigenvalue 1, invariant under Q, is called the axis of rotation. It is easily seen that Q rotates the plane perpendicular to $\underline{x}$ by angle ϕ.
- The direction of $\underline{x}$ is easily found from Q: since $Q\underline{x} = \underline{x}$ and $Q^T\underline{x} = \underline{x}$, it follows that $(Q - Q^T)\underline{x} = 0$. Then

$$\frac{x_1}{Q_{32} - Q_{23}} = \frac{x_2}{Q_{13} - Q_{31}} = \frac{x_3}{Q_{21} - Q_{12}} \ .$$

Returning to the discussion of the previous section, we see now how to construct the quaternion associated with a given rotation matrix: simply set

$$q = \pm\left(\cos(\theta/2), \sin(\theta/2)\underline{x}\right) \ ,$$

assuming $|\underline{x}| = 1$.

For the reverse construction, i.e. for the matrix representation of a given quaternion (that is, for finding the matrix that affects a rotation about an axis $\underline{x}$ by angle θ in 3-space, we proceed directly: assume $q = (q_0, \underline{q}) \in \mathcal{Q}_1$, $\underline{q} = q_1 e_1 + q_2 e_2 + q_3 e_3$. Then, from $r' = qrq^c$ we can determine the matrix that transforms the components of a given vector $r = (0, \underline{r})$ to those of $r' = (0, \underline{r}')$. We have:

$$\begin{aligned} (0, \underline{r}') &= (q_0, \underline{q})(0, \underline{r})(q_0, -\underline{q}) \\ &= (-\underline{q}\cdot\underline{r}, q_0\underline{r} + \underline{q}\times\underline{x})(q_0, -\underline{q}) \\ &= (0, (q_0^2 - \underline{q}\cdot\underline{q})\underline{r} + 2\underline{q}(\underline{q}\cdot\underline{r}) + 2q_0\underline{q}\times\underline{r}) \end{aligned}$$

giving

$$\underline{r}' = \mathbf{A}\underline{r}$$

with

$$\mathbf{A} = (q_0^2 - \underline{q}\cdot\underline{q})\mathbf{I} + 2\underline{q}\underline{q}^T + 2q_0 \begin{pmatrix} 0 & -q_3 & q_2 \\ q_3 & 0 & -q_1 \\ -q_2 & q_1 & 0 \end{pmatrix}$$

or

$$\mathbf{A} = 2 \begin{pmatrix} (q_0^2 + q_1^2 - q_2^2 - q_3^2)/2 & q_1q_2 - q_0q_3 & q_1q_3 + q_0q_2 \\ q_1q_2 + q_0q_3 & (q_0^2 - q_1^2 + q_2^2 - q_3^2)/2 & q_2q_3 - q_0q_1 \\ q_1q_3 - q_0q_2 & q_2q_3 + q_0q_1 & (q_0^2 - q_1^2 - q_2^2 + q_3^2)/2 \end{pmatrix} .$$

If we set $q_0 = \cos(\theta/2)$, $q_i = \sin(\theta/2)x_i$, $x_1^2 + x_2^2 + x_3^2 = 1$, then we can write

$$\mathbf{A} = \cos\theta\mathbf{I} + (1 - \cos\theta)\begin{pmatrix} x_1^2 & x_1x_2 & x_1x_3 \\ x_2x_1 & x_2^2 & x_2x_3 \\ x_3x_1 & x_3x_2 & x_3^2 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}$$

where $\underline{x}$ is the axis and θ the angle of rotation. As $\mathbf{A}$ is quadratic in q, using $\pm q$ give the same result.

7 Translations in Q and the groups $SU(2,\mathbf{C})$ and $SO(4,\mathbf{R})$.

We now consider another representation of the quaternions, intended to clarify the composition of rotations. To simplify the discussion, we consider quaternions of the form: $z = a_0e_0 + a_1e_1$ and identify them with the complex numbers:

$$z = a_0e_0 + a_1e_1 \sim a_0 + a_1 i \ .$$

Then the arbitrary quaternion q can be written :

$$q = \sum_0^3 a_i e_i = e_0 z + e_2 w$$

where z is as above and $w = a_2e_0 - a_1e_1$. In what follows we use the symbol for the imaginary unit, i, interchangeably with e_1, i.e. $e_2 i = -ie_2 = -e_3$ etc. Define now the translation operator T_q :

$$T_q(v) := qv \ .$$

In components, and using the obvious fact $we_2 = e_2 w^\star$ (where $z^\star$ is the normal complex conjugate) it is not hard to see that, with $v = e_0 s + e_2 u$,

$$T_q(v) = qv = (e_0 z + e_2 w)(e_0 s + e_2 u) = e_0(zs - w^\star u) + e_2(ws - z^\star u)$$

so that, if we identify the quaternion $v = e_0 s + e_2 u$ with the complex 2-vector $(s,u)^T$ and we restrict to $q \in \mathcal{Q}_1$ we see that the mapping

$$q \to T_q = \begin{pmatrix} z & -w^\star \\ w & z^\star \end{pmatrix}$$

provides a faithful representation of the group of unit quaternions $\mathcal{Q}_1$ into the group $SU(2,\mathbf{C})$ of 2×2 unitary complex matrices:

$$T_q T_p = T_{qp}$$

and

$$det(T_q) = |z|^2 + |w|^2 = N(q) = 1 \ .$$

Since all elements of $SU(2,\mathbf{C})$ can be thus constructed and the correspondence is 1-1, it follows that $q \to T_q$ is a group isomorphism of $\mathcal{Q}_1$ with $SU(2,\mathbf{C})$.

Returning to quaternions, we now construct the composition of rotations in terms of unitary matrices. A more useful representation, in terms of real 4X4 orthogonal matrices can be found by direct multiplication: if $q = (a_0, \underline{a})$, $v = (b_0, \underline{b})$ then

$$T_q(v) = qv = (a_0b_0 - \underline{a}\cdot\underline{b}, a_0\underline{b} + b_0\underline{a} + \underline{a}\times\underline{b})$$

and writing $v = (b_0, b_1, b_2, b_3)^T$ we find:

$$T_q = \begin{pmatrix} a_0 & -a_1 & -a_2 & -a_3 \\ a_1 & a_0 & -a_3 & a_2 \\ a_2 & a_3 & a_0 & -a_1 \\ a_3 & -a_2 & a_1 & a_0 \end{pmatrix} .$$

If $q \in \mathcal{Q}_1$, this is easily seen to be an orthogonal transformation in $\mathbf{R}^4$.

8 Rigid body dynamics: The use of quaternions in the numerical integration of the Euler equations.

An application of the quaternion reduction for rotations is discussed for the solution of the Euler equations of motion of a rigid body with one point fixed in three dimensional space. The natural setting for describing the motion are the "body-fixed coordinates" in which the moment of inertia tensor is constant. In the absence of externally applied torques, the motion is integrable and the angular velocity (and momentum) can be determined explicitly for all time in terms of elliptic functions. However, to produce a description of the motion in space, we need to compute the orthogonal transformation that relates to the "Space-fixed" coordinate system. This requires the computation of an evolving orthogonal matrix from the time history of the angular velocity. This computation is much simpler in the quaternion representation. Moreover, if an external torque is applied, its description in body coordinates requires knowledge of the orthogonal transformation. In that case the two sets of equations become coupled, and apart from a few special cases, the Euler equations are no longer integrable in general.

8.1 The Euler equations for rigid body dynamics.

A rigid body is a system of points whose mutual distances are fixed in space. In the following discussion we shall assume that one of the points of a rigid body, O, is fixed in space, and we shall introduce two orthogonal coordinate systems: an inertial coordinate system $Ox_1x_2x_3$, fixed in space, and the system $OX_1X_2X_3$ fixed in the body. We shall choose the body system so that it's axes coincide with the principal axes of inertia. In the following discussion we shall adopt the notation of, and refer to, Arnold's *Mathematical Methods of Classical Mechanics*, Chapter 6 ([1]).

In the sequel we shall use $\mathbf{x}$ to denote a vector, $\underline{x}$ to denote its coordinates in space and $\underline{X}$ to denote its coordinates in the body. In keeping track of the motion of a rigid body, one needs to be able to give its orientation is space at each instant. A vector $\underline{X}$ in the body will have coordinates in space

$$\underline{x} = Q(t)\underline{X}$$

where $Q(t)$ is an orthogonal transformation. For the time evolution of $\underline{X}$ and $\underline{x}$ we have:

$$\frac{d\underline{x}}{dt} = \frac{dQ}{dt}\underline{X} + Q\frac{d\underline{X}}{dt} \ .$$

Since $\underline{X} = Q^T\underline{x}$ we can write

$$\frac{d\underline{x}}{dt} = \frac{dQ}{dt}Q^T\underline{x} + Q\frac{d\underline{X}}{dt} \ .$$

Since $QQ^T = I$, it follows that the matrix $Q'Q^T$ is skew symmetric, so that there exists a vector $\underline{\omega}$ such that

$$s(t) := Q'Q^T = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \tag{1}$$

so that

$$\underline{x}' = [\underline{\omega}, \underline{x}] + Q\underline{X}' \ . \tag{2}$$

The vector $\underline{\omega}$ is called the instantaneous angular velocity in space. In the body, eq.(2) is written, using the invariance of the cross-product (i.e. the fact that $[\underline{\omega}, \underline{x}] = [Q\underline{\Omega}, Q\underline{X}] = Q\,[\underline{\Omega}, \underline{X}]$):

$$\underline{x}' = Q\left([\underline{\Omega}, \underline{X}] + \underline{X}'\right) \ . \tag{3}$$

The angular momentum $\underline{m}$ ($\underline{M} = Q^T\underline{m}$ in the body) of a rigid body is related to its angular velocity by the inertia tensor, $\mathcal{A}$:

$$\underline{m} = \mathcal{A}|_{\text{space}}\underline{\omega}$$

with a similar equation for body quantities. By choosing its principal axes for our body coordinate system, we can write $\mathcal{A}$ in the form

$$\mathcal{A}|_{\text{body}} =: A = I_1 e_1 e_1^T + I_2 e_2 e_2^T + I_3 e_3 e_3^T \ .$$

This expression is, of course, constant, while $\mathcal{A}|_{\text{space}} =: a(t) = Q(t)AQ^T(t)$ varies, depending on the body's orientation. The matrix A is symmetric, positive semidefinite, and we assume that $0 < I_1 \geq I_2 \geq I_3 \geq 0$. The kinetic energy is easily seen to be

$$T(\underline{\omega}) = T(\underline{\Omega}) = \frac{1}{2}\left(\underline{M}, \underline{\Omega}\right) = \frac{1}{2}\left(A\underline{\Omega}, \underline{\Omega}\right) \ .$$

Newton's laws give

$$\frac{d\underline{m}}{dt} = \underline{t} \ ,$$

with $\underline{t}$ some externally applied torque (which we will assume is a given vector in space). In the body, this becomes:

$$\frac{d\underline{m}}{dt} = \underline{t} = Q\left([\underline{\Omega}, \underline{M}] + \frac{d\underline{M}}{dt}\right) \tag{4}$$

or, rewriten entirely in terms of body variables:

$$\frac{d\underline{M}}{dt} = [\underline{M}, \underline{\Omega}] + \underline{T} \tag{5}$$

with $\underline{T} = Q^T \underline{t}$. These are the Euler equations of motion of a rigid body, one of whose points is fixed in space. In the absense of external torques, there are two integrals: the energy $T(\underline{\Omega})$ and the total angular momentum $M = \underline{M}\cdot\underline{M} = \underline{m}\cdot\underline{m}$, that is

$$\begin{aligned} T &= \frac{1}{2}\left(\frac{M_1^2}{I_1} + \frac{M_2^2}{I_2} + \frac{M_3^2}{I_3}\right) \\ M^2 &= M_1^2 + M_2^2 + M_3^2 \end{aligned}$$

so that the equations are completely integrable and the motion (in the body frame!) happens on the intersection of a sphere and a triaxial ellipsoid. It is clear then that, on the surface of the energy ellipsoid in angular momentum space, the points of intersection of the major and minor axes are centers, while the points of intersection of the intermediate axis are saddlepoints, and motion about that axis is unstable. Of course, the description in space coordinates is considerably more complex.

When torque is included, only a few special cases are known to be integrable, and the problem is hard in all cases ([2]). Here we will focus on aspects related to the numerical integration of (5). For that, we see that the key problem is determining the transformation matrix $Q(t)$ from knowledge of the angular velocity, $\underline{\Omega}$. Indeed, the Euler equations can be readily written in terms of the angular velocity: since $M_i = I_i\Omega_i$, (5) become, in terms of components:

$$\frac{d}{dt}\begin{pmatrix} \Omega_1 \\ \Omega_2 \\ \Omega_3 \end{pmatrix} = \begin{pmatrix} \frac{I_2 - I_3}{I_1}\Omega_2\Omega_3 + \frac{T_1}{I_1} \\ \frac{I_3 - I_1}{I_2}\Omega_3\Omega_1 + \frac{T_2}{I_2} \\ \frac{I_1 - I_2}{I_3}\Omega_1\Omega_2 + \frac{T_3}{I_3} \end{pmatrix} \tag{6}$$

with $\underline{T} = Q^T \underline{t}$.

To completely determine the system in space, we must also determine the operator $Q(t)$ whose evolution is connected to the angular velocity $\underline{\Omega}$ by the equation

$$\frac{dQ}{dt} = sQ = QS := Q\begin{pmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & \Omega_1 & 0 \end{pmatrix}.$$

However, integration of this system of nine equations in the components of $Q(t)$ is both computationally costly, and may introduce unnecessary errors in that the orthogonality of the rows of Q may not be preserved sufficiently accurately. Instead, we can employ the quaternion representation of rotations, to reduce this computation to an integration of four equations.

8.2 Kinematics: computing the transformation $Q(t)$ from the history of $\Omega(t)$

As we saw previously, for $q \in \mathcal{Q}_1$ (i.e. $N(q) = 1$) the coordinates of a vector in space and body coordinates will be given by

$$x = qXq^c \ , \tag{7}$$

where $x = (0, \underline{x})$, $X = (0, \underline{X})$, and $q = q(t)$ is the quaternion representing a rotation by the matrix $Q(t)$. Then, for $dX/dt = 0$:

$$\frac{dx}{dt} = \frac{dq}{dt}Xq^c + qX\frac{dq}{dt} = \left(\frac{dq}{dt}q^c\right)x + x\left(q\frac{dq^c}{dt}\right) \ .$$

Lemma 1 $\frac{dq}{dt}q^c$ *is a pure quaternion.*

Indeed, the scalar part is (setting $q = (q_0, \underline{q})$): $\frac{dq_0}{dt}q_0 + \frac{d\underline{q}}{dt} \cdot \underline{q} = \frac{d}{dt}N(q) = 0$.

We introduce $v = \frac{dq}{dt}q^c = (0, \underline{v})$. Then, since $v^c = -v$ and $x^c = -x$, we have

$$\frac{dx}{dt} = vx - xv = 2v \times x$$

or, equivalently,

$$\frac{d\underline{x}}{dt} = [2\underline{v}, \underline{x}] \ .$$

In terms of the discussion in the previous subsection, we set

$$\omega = 2v = 2\frac{dq}{dt}q^c \ .$$

This gives the equation (refering to the matrix for multiplication by a quaternion derived at the end of Section 7):

$$\frac{dq}{dt} = \frac{1}{2}\omega q = \frac{1}{2}\begin{pmatrix} 0 & -\omega_1 & -\omega_2 & -\omega_3 \\ \omega_1 & 0 & -\omega_3 & \omega_2 \\ \omega_2 & \omega_3 & 0 & -\omega_1 \\ \omega_3 & -\omega_2 & \omega_1 & 0 \end{pmatrix}\begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} \tag{8}$$

that is, an equation for the rotation has been derived in terms of the angular velocity that involves the evolution of four, instead of nine, quantities. In fact, the first of the above equations simply ensures the conservation of the norm of q.

In terms of the angular velocity in the body frame, we have that $\Omega = q^c\omega q$ or $\omega = q\Omega q^c$ so that

$$\frac{dq}{dt} = \frac{1}{2}q\Omega = \frac{1}{2}\begin{pmatrix} 0 & -\Omega_1 & -\Omega_2 & -\Omega_3 \\ \Omega_1 & 0 & \Omega_3 & -\Omega_2 \\ \Omega_2 & -\Omega_3 & 0 & \Omega_1 \\ \Omega_3 & \Omega_2 & -\Omega_1 & 0 \end{pmatrix}\begin{pmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} \tag{9}$$

which, together with the Euler equations for Ω

$$\frac{d}{dt}\begin{pmatrix}\Omega_1\\ \Omega_2\\ \Omega_3\end{pmatrix} = \begin{pmatrix}\frac{I_2-I_3}{I_1}\Omega_2\Omega_3+\frac{T_1}{I_1}\\ \frac{I_3-I_1}{I_2}\Omega_3\Omega_1+\frac{T_2}{I_2}\\ \frac{I_1-I_2}{I_3}\Omega_1\Omega_2+\frac{T_3}{I_3}\end{pmatrix} \tag{10}$$

and the equations giving the torque in the body frame from its space frame value

$$(0,\underline{T}) = q^c(0,\underline{t})q \rightarrow \underline{T} = Q^T\underline{t}$$

where the rotation matrix, Q, is given in terms of the components of q by

$$Q = 2\begin{pmatrix}(q_0^2+q_1^2-q_2^2-q_3^2)/2 & q_1q_2-q_0q_3 & q_1q_3+q_0q_2\\ q_1q_2+q_0q_3 & (q_0^2-q_1^2+q_2^2-q_3^2)/2 & q_2q_3-q_0q_1\\ q_1q_3-q_0q_2 & q_2q_3+q_0q_1 & (q_0^2-q_1^2-q_2^2+q_3^2)/2\end{pmatrix}.$$

Finally, the position of a point in the body, $\underline{X}$, in terms of absolute space coordinates is given by the transformation

$$(0,\underline{x}) = q(0,\underline{X})q^c \rightarrow \underline{x} = Q\underline{X}\ .$$

Variants of the above form of the rigid body equations, with a time integration involving the three components of the angular velocity and the four components of q have been used by various authors in the numerical integration of the equations describing non-Newtonian fuids such as liquid crystals, molecular dynamics simulations of complex molecules etc. (see, eg., [3], [5]).

Acknowledgment In preparing these notes, we made use of the lecture notes of Prof. Paco A. Lagerstrom on quaternions and representations of the rotation group ([4]).

References

[†] vageli@math.unm.edu

[‡] laromer@chimayo.sandia.gov

[1] V.I. Arnol'd, *Mathematical Methods of Classical Mechanics* , 2nd ed., Springer, New York, 1992.

[2] M. Aubin, *Tops*, Cambridge Univ. Press, (1994).

[3] J. Billeter and R. Pelcovits, Simulations of liquid crystals, *Computers in Physics* v.12, No.5, p.440-448 (1998).

[4] P.A. Lagerstrom, *AMa 251: Applications of Group Theory* , class notes, Caltech, 1973 (unpublished).

[5] Rappaport, D.C., *The Art of Molecular Dynamics Simulation* , Cambridge Univ. Press, New York, Chapter 8, pp. 191-221, 1995.

[6] I.M. Yaglom, *Felix Klein and Sophus Lie: Evolution of the Idea of Symmetry in the Nineteenth Century*, Birkhäuser, Boston (1988).