QUATERNION PARAMETER ALGORITHMS

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Introduction

There has been a steady growth of interest in recent years in the use of quaternion parameters to represent rigid body orientations in classical mechanics. Of most relevance here, of course, are the molecular dynamics algorithms based on quaternion parameters |1|, which are represented in the CCP5 program library |2|, but the wider interest is clearly shown by the discussion, in some detail, of quaternions in the second edition of Goldstein's text 'Classical Mechanics' |3|. In this article, I wish to summarize the orientational equations of motion, as concisely as possible, in quaternion form, and to draw attention to a way of integrating them which, I believe, has not been studied extensively. This approach may be most useful when the interaction potentials are simply expressed in terms of the quaternions themselves (multipole-multipole interactions are an example). Some of the discussion will be restricted to the case of spherical top molecules, for simplicity, but it should be clear how to extend the treatment to the general case. Much of this material will be familiar to many readers, and I make no great claims of originality as regards this general approach.

Quaternion parameter notation

I will use lower case symbols to represent scalars and vectors, and upper case for quaternions:

$$Q = (q_0, q_1, q_2, q_3) = (q_0, \vec{q}) \tag{1}$$

I follow Goldstein in numbering the four scalar components of the quaternion from zero. As indicated here, the triple (q_1, q_2, q_3) may often be regarded as a vector $\vec{q}$ in 3D space. Quaternion "multiplication" is defined:

$$P*Q = (p_0q_0 - \vec{p}\cdot\vec{q},\ p_0\vec{q} + q_0\vec{p} - \vec{p}\times\vec{q}) \tag{2}$$

This operation is not commutative, so $Q*P \neq P*Q$, but it _is_ associative, so we can unambiguously write $P*Q*R = P*(Q*R) = (P*Q)*R$. This last property is in contrast to the vector cross product $\vec{p}\times\vec{q}$ which appears in equation (2). Addition of two quaternions, and multiplication of a quaternion by a scalar, are both simple component-by-component operations. The conjugate of Q is written $\tilde{Q}$:

$$\tilde{Q} = (q_0, -\vec{q}) \tag{3}$$

so that

$$\tilde{Q}*Q = Q*\tilde{Q} = (|Q|^2, \vec{0}) \tag{4}$$

Here, $\vec{0}$ is the null vector, and the norm $|Q|^2$ is defined

$$|Q|^2 = q_0^2 + q_1^2 + q_2^2 + q_3^2 \tag{5}$$

For a quaternion Q with _unit_ norm, $\tilde{Q}$ is the same as Q^{-1}, the inverse of Q, since the resultant $\tilde{Q}*Q = (1, \vec{0})$ acts as an identity element.

Goldstein discusses the way in which a quaternion Q with unit norm may represent the orientation of a rigid body, and clarifies the relationship between the components of Q and the Euler angles $(\phi\theta\psi)$ in various conventions. The rotation matrix $\bar{\bar{A}}$, defined by

$$\vec{r}^{\,b} = \bar{\bar{A}}\,\vec{r}^{\,s} \tag{6}$$

where $\vec{r}^{\,b}$ and $\vec{r}^{\,s}$ are the components of a vector in body-fixed and space-fixed coordinate systems, respectively, can invariably be written in the symmetrical form:

$$\bar{\bar{A}} = \begin{pmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2(q_1q_2+q_0q_3) & 2(q_1q_3-q_0q_2) \\ 2(q_1q_2-q_0q_3) & q_0^2-q_1^2+q_2^2-q_3^2 & 2(q_2q_3+q_0q_1) \\ 2(q_1q_3+q_0q_2) & 2(q_2q_3-q_0q_1) & q_0^2-q_1^2-q_2^2+q_3^2 \end{pmatrix} \qquad (7)$$

To achieve this, one should choose a definition of Q which is consistent with the Euler angle convention employed (this has not always been the case in the past). For example, in the 'y-convention' |4|, the definitions

$$\begin{aligned} q_0 &= \cos\tfrac{1}{2}(\psi+\phi)\cos\tfrac{1}{2}\theta \\ q_1 &= \sin\tfrac{1}{2}(\psi-\phi)\sin\tfrac{1}{2}\theta \\ q_2 &= \cos\tfrac{1}{2}(\psi-\phi)\sin\tfrac{1}{2}\theta \\ q_3 &= \sin\tfrac{1}{2}(\psi+\phi)\cos\tfrac{1}{2}\theta \end{aligned} \qquad (8)$$

yield equation (7). With such a choice, as is well-known, the rotation from body-fixed to space-fixed coordinates can be expressed as a quaternion operation. Defining quaternions $R^b = (0, \vec{r}^b)$, $R^s = (0, \vec{r}^s)$, equations (6), (7) are equivalent to

$$R^b = \tilde{Q}*R^s*Q \qquad (9)$$

Equations of motion

The orientational equations of motion, in quaternion form, may be derived by straightforward but tedious trigonometry applied to the time derivative $\dot{Q}$, or by considering the time-evolution of $\bar{\bar{A}}$. The result is usually expressed in terms of a 4×4 matrix acting on the four components of an angular velocity quaternion $\Omega^b = (0, \vec{\omega}^b)$ (body-fixed) or $\Omega^s = (0, \vec{\omega}^s)$ (space-fixed), but is most compactly written:

$$\dot{Q} = \tfrac{1}{2}Q*\Omega^b = \tfrac{1}{2}\Omega^s*Q \qquad (10)$$

For a spherical top, the time derivative of the angular velocity is given by

$$\dot{\Omega}^b = N^b \qquad\qquad \dot{\Omega}^s = N^s \tag{11}$$

where $N^b = (0, \vec{n}^b)$, $N^s = (0, \vec{n}^s)$, and $\vec{n}^b$ and $\vec{n}^s$ are the body-fixed and space-fixed components, respectively, of the applied torque, divided by the moment of inertia.

Consider how these equations are integrated. Typically, (e.g. in the CCP5 program library) equations (10) and (11) are treated using a pair of (say) 4th order predictor-corrector procedures, coupled together:

(a) PREDICT the new values of Q, $\dot{Q}$,..$Q^{(4)}$ from current values of Q, $\dot{Q}$ etc.;

(b) PREDICT the new values of Ω^b, $\dot{\Omega}^b$,..$\Omega^{b^{(4)}}$ from current values of Ω^b etc.;

(c) EVALUATE N^b from the predicted Q;

(d) CORRECT the values of Ω^b, $\dot{\Omega}^b$ etc., using N^b (equation (11));

(e) EVALUATE $\frac{1}{2}Q*\Omega^b$ from the corrected Ω^b and the predicted Q;

(f) CORRECT the values of Q, $\dot{Q}$ etc., using $\frac{1}{2}Q*\Omega^b$ (equation (10)).

This sequence is generally followed by a renormalization of Q to counteract the cumulative effects of algorithm error (hopefully small!). The predictor steps will generally be sinple Taylor series, while the corrector will be the Gear formula |5| appropriate for a first order differential equation, (10) or (11).

This approach has been shown to work well. Dealing with body-fixed angular velocities and torques is necessary if the approach is to handle, in a natural way, non-spherical molecules. The angular velocities are available for the computation of kinetic energy. Other beneficial features will be mentioned later. However, one obvious feature, in view of equation (10), is that a lot of redundant information is being stored in the form of Q, Ω^b, and the first 4 time derivatives of both. Remember that one main idea behind the quaternion approach was to obtain equations of motion which are not singular (as the Euler equations are) without going so far as to store (for example) all 9 components of the rotation matrix, plus derivatives.

My interest here is with the alternative method, namely the elimination of the angular velocities from equations (10) and (11) to yield a single, second-order, equation of motion. For a spherical top, the result is the same whether one starts from the body-fixed or space-fixed forms of (10), (11), and is

$$\ddot{Q} = \dot{Q}*\tilde{Q}*\dot{Q} + \tfrac{1}{4}N \tag{12}$$

The second derivative $\ddot{Q}$ contains a "kinetic" part, but the more interesting term is N which can be expressed in terms of body-fixed or space-fixed torques:

$$N = 2Q*N^b = 2N^s*Q \tag{13}$$

The chain rule for differentiation shows that N is actually a quaternion "force" or "torque", and can be expressed

$$N = -(\partial V/\partial q_0,\ \partial V/\partial q_1,\ \partial V/\partial q_2,\ \partial V/\partial q_3) \tag{14}$$

where V is the potential energy and the derivatives $\partial/\partial q_i$ may be taken holding the other 3 quaternions constant (see below). The situation for non-spherical molecules is only slightly more complex, in that at some stage the torque must be expressed in body-fixed coordinates so as to divide out the principal moments of inertia.

The suggestion, then, is that equation (12) may be integrated directly, using equation (13) or (14) for N. Any algorithm suitable for general second-order differential equations could be employed, as long as it does not demand the absence of time derivatives of Q on the right; the Gear methods would be appropriate for instance. The scheme would be:

(a) PREDICT the new values of Q, $\dot{Q}$,... from their current values;

(b) EVALUATE the right hand side of equation (12) as a function $F(Q,\dot{Q})$;

(c) CORRECT the values of Q, $\dot{Q}$,... using $F(Q,\dot{Q})$ (equation (12)).

Only the quaternions Q and their time derivatives need be stored; probably 5 derivatives would be needed to achieve an accuracy comparable with the pair of 4th order algorithms mentioned above. There would be no need to store angular velocities, Euler angles, direction cosines or rotation matrices; the angular velocities could be obtained from equation (10) and the kinetic energy would be given by $\frac{1}{2}I\omega^{s^2} = \frac{1}{2}I\omega^{b^2} = 2I|\dot{Q}|^2$.

Now for the caveats. The astute reader will already have noticed that the torque N is not completely defined by equation (14), since V is actually a function of 3 independent angular parameters, not 4. In fact, because Q has unit norm, we could add any function of the form $\frac{1}{2}f(q_0,q_1,q_2,q_3)\times(q_0{}^2+q_1{}^2+q_2{}^2+q_3{}^2-1)$ to V, without changing its value, but thereby replacing N in equation (14) by N+fQ. The extra term simply affects the time evolution of the <u>norm</u> of Q. Remembering that $|Q|^2 = 1$, we have

$$\partial/\partial t \quad (|Q|^2) = 2(\tilde{Q}*\dot{Q})_0 = 2(q_0\dot{q}_0+q_1\dot{q}_1+q_2\dot{q}_2+q_3\dot{q}_3) = (\Omega^b)_0 = (\Omega^s)_0 = 0 \qquad (15a)$$

$$\partial^2/\partial t^2 \quad (|Q|^2) = \tfrac{1}{2}(\tilde{Q}*N)_0 = \tfrac{1}{2}(q_0n_0+q_1n_1+q_2n_2+q_3n_3) = (N^b)_0 = (N^s)_0 = 0 \qquad (15b)$$

where $(\ldots)_0$ means "zeroth component of". Both of these quantities should be zero. Since the CCP5 implementation makes use of body-fixed angular velocity and torque components, equations (15a), (15b) are <u>guaranteed</u>, that is the norm remains constant to at least second order. Equation (15b) will also be obeyed in the integration of equation (12) if we obtain N from N^s or N^b, <u>via</u> equation (13). The problem arises if we use equation (14) for N, when the differentiation should really be carried out <u>subject to</u> the condition (15b). In practice it is simpler (and equivalent) to take unconstrained derivatives, as suggested above, and then correct N. This can be done by transforming N to N^b (equation (13)), setting $n_0^b = 0$, dividing n_1^b, n_2^b, n_3^b by the principal moments of inertia in the non-spherical case (since this is a convenient point to do it) and then transforming back to N. Alternatively, in the case of the spherical top, we could simply compute the projection $f = q_0n_0+q_1n_1+q_2n_2+q_3n_3$ and then replace N by N-fQ. A similar procedure would be used to ensure that equation (15a) is satisfied: compute $f' = q_0\dot{q}_0+q_1\dot{q}_1+q_2\dot{q}_2+q_3\dot{q}_3$ and replace $\dot{Q}$ by $\dot{Q}$-f'Q. I believe that these procedures are no less important, for the integration of equation (12), than the simple rescaling of Q to guarantee unit norm. The reader may like to consider whether similar corrections should be applied to the third and higher derivatives of Q.

I have conducted preliminary runs for single-particle and for many-particle systems of rotors pinned to lattice sites, comparing the direct integration of equation (12) (by 5th order Gear algorithm for 2nd order differential equations) with the integration of equations (10) and (11) (by a pair of 4th order Gear algorithms for 1st order differential equations). In each case, point multipole potentials (expressed as simple polynomials of the quaternion parameters) were used, and N obtained *via* equation (14). The direct method looks promising in this particular application, but only becomes competitive (as far as energy conservation is concerned) when the corrections suggested above are incorporated at each time step; otherwise the "zeroth components" of torque and angular velocity in the body-fixed frame soon build up. Merely correcting the torque is itself insufficient: the time derivative $\dot{Q}$ must be made "orthogonal" to Q, to prevent the accumulation of error during the run.

Conclusion

It is possible to integrate the orientational equations of motion, in quaternion form, directly, i.e. as second order differential equations. This approach would be useful when the potential energy can be easily expressed in terms of the quaternions themselves, and it saves a little on storage compared with the usual treatment, as a pair of first order differential equations. The way in which the direct approach deals with non-spherical molecules, and the corrections which must be applied to ensure that time derivatives of the norm $|Q|^2$ are zero, are less elegant than the corresponding features of the normal method, but are not particularly time-consuming. Any comments?

References

1 EVANS, D. J., MURAD, S., Molec. Phys. 34 327 (1977).

2 THOMPSON, S. M., descriptions of CCP5 programs HMDIAT, MDLIN, MDTETRA etc.

3 GOLDSTEIN, H., 'Classical Mechanics', 2nd edition (Addison-Wesley, 1980).

4 Beware a minor typographical error on p607 of reference 3. In equation (B-3y), bottom row of rotation matrix, ψ should be replaced by ϕ.

5 GEAR, C. W., 'Numerical Initial Value Problems in Ordinary Differential Equations', (Prentice Hall, 1971).