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Family of Constraint-Preserving Integrators for Solving Quaternion Equations

J. C. Chiou* and Y. W. Jan†
National Chiao Tung University, Hsinchu 30010, Taiwan, Republic of China
and
S. D. Wu‡
Precision Instrument Development Center, Hsinchu 30010, Taiwan, Republic of China

A family of numerical time integrators that exactly preserve the constraint of quaternion equations is developed. The constraint-preserving integrators based on the property of the skew-symmetric matrix and the proposed proven theorems are used to improve the accuracy of updating Euler parameters. The stability and accuracy analysis of the generalized constraint-preserving integrators is also discussed. Furthermore, we demonstrate that the proposed integrators are A-stable integrators that are proven to be useful in calculating angular orientations of kinematic and dynamic systems. A numerical example is used to demonstrate the superiority of the proposed integrators.

I. Introduction

To avoid degeneration of the coordinate transformation matrix, Euler parameters have frequently been chosen to present the angular orientations of the body for the reasons that Euler parameters 1) satisfy the singularity free property, 2) preserve the algebraic description of finite rotation, and 3) simplify the mathematical formulation. An accurate and efficient algorithm in updating Euler parameters plays an important role in computing attitude from inertial measurement unit data. Euler parameters are generalized coordinates of angular orientation of a reference frame $\boldsymbol{e}_1$ with respect to another reference frame $\boldsymbol{e}_2$. If these two frames coincide initially, we let the $\boldsymbol{e}_2$ frame rotate about an axis unit $\boldsymbol{n}$ through an angle ϕ. The two frames have the following relationship after the rotation[1]:

$$\boldsymbol{e}_2 = R\boldsymbol{e}_1 \tag{1}$$

where the rotation matrix R is defined as

$$R = 2\begin{bmatrix} q_0^2 + q_1^2 - \frac{1}{2} & q_1q_2 + q_0q_3 & q_1q_3 - q_0q_2 \\ q_1q_2 - q_0q_3 & q_0^2 + q_2^2 - \frac{1}{2} & q_2q_3 + q_0q_1 \\ q_1q_3 + q_0q_2 & q_2q_3 - q_0q_1 & q_0^2 + q_3^2 - \frac{1}{2} \end{bmatrix} \tag{2}$$

The quantities q_i ($i = 0, 1, 2, 3$) are called Euler parameters and are defined as

$$q_0 = \cos(\phi/2) \tag{3a}$$

$$q_i = n_i \sin(\phi/2), \qquad i = 1, 2, 3 \tag{3b}$$

with the constraint

$$\sum_{i=0}^{3} q_i^2 = 1 \tag{4}$$

When the $\boldsymbol{e}_2$ frame is rotating relative to the $\boldsymbol{e}_1$ frame with an angular velocity vector $[\omega_1(t) \;\; \omega_2(t) \;\; \omega_3(t)]^T$, the Euler parameters are obtained by solving the quaternion equations

$$\begin{bmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 0 & -\omega_1(t) & -\omega_2(t) & -\omega_3(t) \\ \omega_1(t) & 0 & \omega_3(t) & -\omega_2(t) \\ \omega_2(t) & -\omega_3(t) & 0 & \omega_1(t) \\ \omega_3(t) & \omega_2(t) & -\omega_1(t) & 0 \end{bmatrix}\begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} \tag{5}$$

Because the closed-form solution of Eq. (5) is unattainable, we must integrate the differential Eq. (5) numerically in order to update the Euler parameters accurately. In the past two decades, researchers have developed many integration algorithms to solve the quaternion equations. These algorithms have ranged from the Runge–Kutta (RK) method,[2,3] which is accurate but time-consuming, to the second-order Adams–Bashforth (AB-2) method,[2,4] which has a low computational cost but is less accurate. To counteract the drawbacks of these two methods, Lawrence et al.[5] developed a local linearization (LL) algorithm to solve the quaternion more effectively. Furthermore, Yen and Cook[6] proposed a new LL algorithm to improve the efficiency of the old LL algorithm. However, regardless of the nature of the algorithms, these algorithms introduce so-called artificial damping into the quaternion equations and cause the constraint equation (4) to be violated during the numerical time integration process. To overcome this difficulty, two modified formulas were proposed to correct the Euler parameters. The first modified method was proposed by Nikravesh and is given as follows[7]:

$$q_i^* = \frac{q_i}{\sqrt{\sum_0^3 q_i^2}} \tag{6}$$

where q_i^* ($i = 0, 1, 2, 3$) denotes the corrected Euler parameters. Nikravesh's modified method was obtained by minimizing the following cost function:

$$\sum_0^3 \left(q_i^* - q_i\right)^2 \tag{7}$$

The four Euler parameters obtained from Eq. (6) are divided by the same quantity so that the correction affects only the rotation angle and not the direction of the rotational axis.[1] In this regard, Wittenburg[1] developed another modified formula to improve this drawback. Instead of minimizing the cost function (7), Wittenburg proposed to minimize the cost function

$$\sum_{i=1}^{3}\sum_{j=1}^{3} \left(R_{ij}^* - R_{ij}\right)^2 \tag{8}$$

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*Professor, Department of Electrical and Control Engineering; chiou@cc.nctu.edu.tw. Member AIAA.
†Graduate Ph.D. Student, Department of Electrical and Control Engineering.
‡Project Research Associate, Research and Develop Division.

which gives the following modified formula:

$$\varepsilon = \sum_{0}^{3} q_i^2 - 1 \tag{9a}$$

$$\mu = \frac{1}{2}\left(1 + \sqrt{1 + 4\varepsilon q_0}\right) + \varepsilon \tag{9b}$$

$$q_0^* = \left[1 + \frac{\left(q_1^2 + q_2^2 + q_3^2\right)q_0^2}{\left(q_1^2 + q_2^2 + q_3^2 - \mu\right)^2}\right]^{-\frac{1}{2}} \tag{9c}$$

$$q_i^* = q_i \frac{q_0 q_0^*}{\mu - \left(q_1^2 + q_2^2 + q_3^2\right)} \tag{9d}$$

As we can imagine, the modified methods given in Eqs. (6) and (9) are not necessary if the developed time integration algorithms are free of artificial damping. In the past decade, many numerical time integrators that possess no artificial damping have been developed to solve separable Hamiltonian systems. These integrators include the partitioned Runge–Kutta methods[8,9] and the symplectic integrators.[10−12] Unfortunately, these integrators cannot be applied directly to solve the quaternion equations because the quaternion equations are inseparable. In 1990, Chiou[13] and Park and Chiou[14] proposed a second-order integrator based on the midpoint and trapezoidal rule to solve the quaternion equations. However, during the development of the integrator, the authors did not show a constraint-preserving property that preserved the constraint equation exactly and automatically. Furthermore, for high-order accuracy in updating Euler parameters, no systematic solution was offered in their derivations. In this regard, the theoretical constraint-preserving property and the high-order constraint-preserving integrators are derived in this paper. Furthermore, we have shown that the present integrators are A-stable (unconditionally stable) integrators.

In the following sections, Sec. II shows the properties involving the skew-symmetric matrix and the quaternion equations. The generalized form of the constraint-preserving integrator is also discussed. Section III presents the stability analysis of the generalized constraint-preserving integrators. We demonstrate that the proposed integrators are A-stable integrators. A family of constraint-preserving integrators is derived in Sec. IV. In Sec. V, a numerical example with time varying angular velocities is used to demonstrate the efficiency and effectiveness of the proposed integrators. The main contribution of this paper is summarized in Sec. VI.

II. Generalized Constraint-Preserving Integrators

In this section, the construction of the generalized constraint-preserving integrators is given. At the beginning, we start with the properties of a specified skew-symmetric matrix S that has the following form:

$$S = \begin{bmatrix} 0 & a & b & c \\ -a & 0 & -c & b \\ -b & c & 0 & -a \\ -c & -b & a & 0 \end{bmatrix} \tag{10}$$

where a, b, and c are any arbitrary scalars. The properties of this specified skew-symmetric matrix are given in Propositions 1–3.

Proposition 1:

$$[[I - S]^{-1}]^T = [I + S]^{-1} \tag{11}$$

where I is the 4×4 identity matrix.

Proof: The inverse of matrix $[I - S]$ can be expanded as follows

$$[I - S]^{-1} = \sum_{n=0}^{\infty} S^n \tag{12}$$

By taking the transpose of

$$\sum_{n=0}^{\infty} S^n$$

one obtains

$$\left(\sum_{n=0}^{\infty} S^n\right)^T = \sum_{n=0}^{\infty} (S^n)^T = \sum_{n=0}^{\infty} (S^T)^n \tag{13}$$

Because S is a skew-symmetric matrix, we have the following relationship:

$$\sum_{n=0}^{\infty} (S^T)^n = \sum_{n=0}^{\infty} (-S)^n = (I + S)^{-1} \tag{14}$$

QED

Proposition 2: If the matrix J is defined by

$$J = [I - S]^{-1}[I + S] \tag{15}$$

then J is an orthonormal matrix that has the following property:

$$J^T J = I \tag{16}$$

Proof: The product of matrix J^T and matrix J is given by

$$J^T J = [I + S]^T [[I - S]^{-1}]^T [I - S]^{-1}[I + S] \tag{17}$$

Because S is a skew-symmetric matrix, one gets

$$J^T J = [I - S][I + S]^{-1}[I - S]^{-1}[I + S] \tag{18}$$

Because matrices $[I - S]$ and $[I + S]^{-1}$ are both polynomials of S, they can be commuted, that is,

$$[I - S][I + S]^{-1} = [I + S]^{-1}[I - S] \tag{19}$$

From Eq. (19), we conclude that

$$J^T J = [I + S]^{-1}[I - S][I - S]^{-1}[I + S] = I \tag{20}$$

QED

Proposition 3:

$$J = [kI - S]^{-1}[kI + S] \tag{21}$$

$$J^T J = I \tag{22}$$

where k is an arbitrary real number.

Proof: The matrix J can be rewritten in the following form:

$$J = [I - (1/K)S]^{-1}[I + (1/k)S] \tag{23}$$

Because matrix $(1/k)S$ has the same form that is shown in Eq. (10), Proposition 3 can be proved directly by using Proposition 2. By using the results of Propositions 1–3, the following theorem is established.

Theorem 1: If an integrator we have used to solve the quaternion equations has the form

$$(kI - S_n)\boldsymbol{q}_{n+1} = (kI + S_n)\boldsymbol{q}_n \tag{24}$$

then

$$\boldsymbol{q}_{n+1}^T \boldsymbol{q}_{n+1} = \boldsymbol{q}_n^T \boldsymbol{q}_n, \qquad \text{for all } n \tag{25}$$

where

$$\boldsymbol{q}_{n+1} = [q_0(n+1), q_1(n+1), q_2(n+1), q_3(n+1)]$$

The matrix S_n shown in Eq. (24) has the following form:

$$S_n = \begin{bmatrix} 0 & a_n & b_n & c_n \\ -a_n & 0 & -c_n & b_n \\ -b_n & c_n & 0 & -a_n \\ -c_n & -b_n & a_n & 0 \end{bmatrix} \tag{26}$$

where parameters a_n, b_n, and c_n are functions of the step size h, the angular velocity $\omega(t)$, and the mth time derivation of $\omega(t)$, respectively.

Proof:

$$q_{n+1} = (kI - S_n)^{-1}(kI + S_n)q_n \equiv J_n q_n \tag{27}$$

$$q_{n+1}^T q_{n+1} = q_n^T J^T J q_n \tag{28}$$

From Proposition 3, we have

$$q_{n+1}^T q_{n+1} = q_n^T q_n$$

QED

Note that Eqs. (24) and (25) provide us with a guideline in deriving the constraint-preserving algorithm. With the propositions and the theorem, we can proceed to discuss the stability of the proposed integrators.

III. Stability Analysis of the Constraint-Preserving Integrators

Stability analysis is the key issue in developing a robust integrator. In this section, the stability of the proposed constraint-preserving integrators is discussed. To begin the discussion, the following proposition is proposed.

Proposition 4:

$$(kI - S)^{-1} = (1/\Delta)(kI + S) \tag{29}$$

where

$$\Delta = k^2 + a^2 + b^2 + c^2 \tag{30}$$

Proof:

$$\begin{bmatrix} k & -a & -b & -c \\ a & k & c & -b \\ b & -c & k & a \\ c & b & -a & k \end{bmatrix}^{-1} = \frac{1}{k^2 + a^2 + b^2 + c^2} \times \begin{bmatrix} k & a & b & c \\ -a & k & -c & b \\ -b & c & k & -a \\ -c & -b & a & k \end{bmatrix} \tag{31}$$

QED

Remark 1: The quantity Δ is equal to the square of norm-2 of any row (column) involved in matrix $(kI + S)$.

From Proposition 4 and Theorem 1, we conclude that the constraint-preserving integrators have the form

$$q_{n+1} = (1/\Delta)(kI + S_n)^2 q_n \equiv J_n q_n \tag{32}$$

Theorem 2: The constraint-preserving integrator described in Eq. (32) is an A-stable (unconditionally stable) integrator.

Proof: The matrix J_n in Eq. (32) can be rewritten as follows:

$$J_n = \frac{1}{\Delta}(kI + S_n)^2 = \begin{bmatrix} K & L & M & N \\ -L & K & -N & M \\ -M & N & K & -L \\ -N & -M & L & K \end{bmatrix} \tag{33}$$

where

$$K = \frac{k^2 - a^2 - b^2 - c^2}{k^2 + a^2 + b^2 + c^2} \tag{34a}$$

$$L = \frac{2ak}{k^2 + a^2 + b^2 + c^2} \tag{34b}$$

$$M = \frac{2bk}{k^2 + a^2 + b^2 + c^2} \tag{34c}$$

$$N = \frac{2ck}{k^2 + a^2 + b^2 + c^2} \tag{34d}$$

The parameters K, L, M, and N involved in J_n satisfy the equality

$$K^2 + L^2 + M^2 + N^2 = 1 \tag{35}$$

The eigenvalues of the transformation matrix J_n are

$$\lambda_1 = \lambda_3 = K + i\sqrt{L^2 + M^2 + N^2} \tag{36a}$$

$$\lambda_2 = \lambda_4 = K - i\sqrt{L^2 + M^2 + N^2} \tag{36b}$$

The magnitude of λ_j ($j = 1, \ldots, 4$) is given by

$$|\lambda_j| = \sqrt{K^2 + L^2 + M^2 + N^2}, \qquad \text{for all } j \tag{37}$$

From Eqs. (35) and (37), we conclude that

$$|\lambda_j| = 1, \qquad \text{for all } j, h, \text{ and } \omega(t) \tag{38a}$$

$$|Re(\lambda_j)| = |K| \le 1, \qquad \text{for all } J \tag{38b}$$

where $Re(\lambda_j)$ is the real part of λ_j. The eigenvalues of matrix J_n lie on or in the unit circle. Thus, we conclude that the proposed integrators are A-stable integrators. QED

In Secs. II and III, the generalized constraint-preserving integrators are derived and the property of A-stability has also been presented. In the next section, the implementation of the constraint-preserving integrators is discussed.

IV. Implementation of Constraint-Preserving Integrators

To implement the constraint-preserving integrators, we need to discuss the property of the skew-symmetric matrix involved in the quaternion equations. The skew-symmetric matrix $A(t)$ is denoted by

$$A(t) = \frac{1}{2}\begin{bmatrix} 0 & -\omega_1(t) & -\omega_2(t) & -\omega_3(t) \\ \omega_1(t) & 0 & \omega_3(t) & -\omega_2(t) \\ \omega_2(t) & -\omega_3(t) & 0 & \omega_1(t) \\ \omega_3(t) & \omega_2(t) & -\omega_1(t) & 0 \end{bmatrix} \tag{39}$$

Proposition 5:

1)

$$A^{2m} = k_m I \tag{40a}$$

where

$$k_m = \left[-\tfrac{1}{4}\left(\omega_1^2 + \omega_2^2 + \omega_3^2\right)\right]^m \tag{40b}$$

and m is an arbitrary positive integer.

2)

$$A^{2m+1} = k_m A \tag{41}$$

Proof:

1)

$$A^2(t) = \frac{1}{4}\begin{bmatrix} 0 & -\omega_1(t) & -\omega_2(t) & -\omega_3(t) \\ \omega_1(t) & 0 & \omega_3(t) & -\omega_2(t) \\ \omega_2(t) & -\omega_3(t) & 0 & \omega_1(t) \\ \omega_3(t) & \omega_2(t) & -\omega_1(t) & 0 \end{bmatrix} \times \begin{bmatrix} 0 & -\omega_1(t) & -\omega_2(t) & -\omega_3(t) \\ \omega_1(t) & 0 & \omega_3(t) & -\omega_2(t) \\ \omega_2(t) & -\omega_3(t) & 0 & \omega_1(t) \\ \omega_3(t) & \omega_2(t) & -\omega_1(t) & 0 \end{bmatrix}$$

$$= -\frac{1}{4}\left[\omega_1^2(t) + \omega_2^2(t) + \omega_3^2(t)\right]^2 I \tag{42}$$

Thus,

$$A^{2m} = \left\{ -\tfrac{1}{4}\left[\omega_1^2(t) + \omega_2^2(t) + \omega_3^2(t)\right]^2 \right\}^m I$$

2) This result can easily be proved using Proposition 5.1.

Proposition 6:

1) The matrix $\dot{A}A - A\dot{A}$ has the same form as S as shown in Eq. (10).

2) The mth time derivation of A, that is, $A^{(m)}$, has the same form as S, which is shown in Eq. (10).

Proof:

1)

$$\dot{A}A - A\dot{A} = \frac{1}{2}\begin{bmatrix} 0 & \omega_3\dot{\omega}_2 - \omega_2\dot{\omega}_3 & \omega_1\dot{\omega}_3 - \omega_3\dot{\omega}_1 & \omega_2\dot{\omega}_1 - \omega_1\dot{\omega}_2 \\ -(\omega_3\dot{\omega}_2 - \omega_2\dot{\omega}_3) & 0 & -(\omega_2\dot{\omega}_1 - \omega_1\dot{\omega}_2) & \omega_1\dot{\omega}_3 - \omega_3\dot{\omega}_1 \\ -(\omega_1\dot{\omega}_3 - \omega_3\dot{\omega}_1) & \omega_2\dot{\omega}_1 - \omega_1\dot{\omega}_2 & 0 & -(\omega_3\dot{\omega}_2 - \omega_2\dot{\omega}_3) \\ -(\omega_2\dot{\omega}_1 - \omega_1\dot{\omega}_2) & -(\omega_1\dot{\omega}_3 - \omega_3\dot{\omega}_1) & \omega_3\dot{\omega}_2 - \omega_2\dot{\omega}_3 & 0 \end{bmatrix} \tag{43}$$

2) It is trivial to prove Proposition 6.2. QED

Proposition 7:

1)

$$\sum_{i=0}^{m} \alpha_i A^{2i} = kI \tag{44}$$

2)

$$\sum_{i=0}^{m} \left[\beta_i A^{2i+1} + \gamma_i A^{(i)}\right] + \delta(\dot{A}A - A\dot{A})$$

has the same form as S, which is shown in Eq. (10).

Proof:

1) By using Proposition 5.

2) By using Propositions 5 and 6. QED

To develop proposed constraint-preserving integrators, first we use the fourth-order Taylor series to approximate the quaternion equations:

$$\begin{aligned} \boldsymbol{q}_{n+1} &= \boldsymbol{q}_n + hA_n\boldsymbol{q}_n + (h^2/2)\left(A_n^2 + \dot{A}_n\right)\boldsymbol{q}_n + (h^3/6)\left(A_n^3 + \ddot{A}_n \right.\\ &\quad \left. + 2\dot{A}_nA_n + A_n\dot{A}_n\right)\boldsymbol{q}_n + (h^4/24)\left(A_n^4 + A_n^2\dot{A}_n + 2A_n\dot{A}_nA_n \right.\\ &\quad \left. + A_n\ddot{A}_n + 3\dot{A}_nA_n^2 + 3\dot{A}_n^2 + 3\ddot{A}_nA_n + \dddot{A}_n\right)\boldsymbol{q}_n + O(h^5) \end{aligned} \tag{45}$$

where $O(\,)$ is the order of the truncation error. By using Theorem 1, we assume that the first-order constraint-preserving integrator has the form

a) First-order constraint-preserving integrator:

$$[I - (h/2)A_n]\boldsymbol{q}_{n+1} = [I + (h/2)A_n]\boldsymbol{q}_n \tag{46a}$$

or

$$\boldsymbol{q}_{n+1} = [I - (h/2)A_n]^{-1}[I + (h/2)A_n]\boldsymbol{q}_n \equiv J_{1,n}\boldsymbol{q}_n \tag{46b}$$

Accuracy analysis: The matrix $J_{1,n}$ can be approximated by

$$J_{1,n} = I + hA_n + (h^2/2)A_n + O(h^3) \tag{47}$$

By comparing the coefficients in Eq. (47) with the coefficients in Eq. (45), we conclude that Eq. (46a) is the first-order constraint-preserving integrator.

b) Second-order constraint-preserving integrator:

The second-order constraint-preserving integrator proposed by Park and Chiou is given next. This integrator is based on the midpoint and trapezoidal rule and is expressed as follows:

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + hA_{n+\frac{1}{2}}\boldsymbol{q}_{n+\frac{1}{2}} \tag{48a}$$

$$\boldsymbol{q}_{n+\frac{1}{2}} = \tfrac{1}{2}(\boldsymbol{q}_{n+1} + \boldsymbol{q}_n) \tag{48b}$$

where

$$A_{n+\frac{1}{2}} = A\left(\omega_{n+\frac{1}{2}}\right) \tag{48c}$$

By combining Eqs. (48a) and (48b), we get

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + (h/2)A_{n+\frac{1}{2}}(\boldsymbol{q}_{n+1} + \boldsymbol{q}_n) \tag{49}$$

Rewriting Eq. (49) yields

$$\left[I - (h/2)A_{n+\frac{1}{2}}\right]\boldsymbol{q}_{n+1} = \left[I + (h/2)A_{n-\frac{1}{2}}\right]\boldsymbol{q}_n \tag{50a}$$

or

$$\boldsymbol{q}_{n+1} = \left[I - (h/2)A_{n+\frac{1}{2}}\right]^{-1}\left[I + (h/2)A_{n+\frac{1}{2}}\right]\boldsymbol{q}_n \equiv J_{2,n}\boldsymbol{q}_n \tag{50b}$$

Accuracy analysis:

$$\begin{aligned} &\left[I - (h/2)A_{n+\frac{1}{2}}\right]^{-1}\left[I + (h/2)A_{n+\frac{1}{2}}\right] \\ &\quad = I + hA_{n+\frac{1}{2}} + (h^2/2)A_{n+\frac{1}{2}} + O(h^3) \end{aligned} \tag{51}$$

Because

$$A_{n+\frac{1}{2}} = A_n + (h/2)\dot{A}_n + O(h^2) \tag{52a}$$

where

$$\dot{A}_n = A(\dot{\omega}_n) \tag{52b}$$

then

$$\begin{aligned} &\left[I - (h/2)A_{n+\frac{1}{2}}\right]^{-1}\left[I + (h/2)A_{n+\frac{1}{2}}\right] \\ &\quad = I + hA_n + (h^2/2)\left(A_n^2 + \dot{A}_n\right) + O(h^3) \end{aligned} \tag{53}$$

By comparing the coefficients involved in Eq. (53) with the coefficients in Eq. (45), we conclude that the Park–Chiou integrator is a second-order integrator. Note that both $(h/2)A_n$ and $(h/2)A_{n+1/2}$ have the form shown in Eq. (10). From Theorems 1 and 2, we conclude that the proposed first-order integrator and Park–Chiou integrator are both A-stable constraint-preserving integrators.

In practical applications, numerical integrators with high-order accuracy may be needed. To improve the accuracy of the Park–Chiou integrator, based on Theorem 1, the third- and fourth-order constraint-preserving integrators are derived and given as follows:

c) Third-order integrator:

$$(\Pi_{3,n} - \Omega_{3,n})\boldsymbol{q}_{n+1} = (\Pi_{3,n} + \Omega_{3,n})\boldsymbol{q}_n \tag{54a}$$

or

$$\boldsymbol{q}_{n+1} = (\Pi_{3,n} - \Omega_{3,n})^{-1}(\Pi_{3,n} + \Omega_{3,n})\boldsymbol{q}_n \equiv J_{3,n}\boldsymbol{q}_n \tag{54b}$$

where

$$\Pi_{3,n} = I + (h/12)A_{n+\alpha}^2 \tag{54c}$$

$$\begin{aligned} \Omega_{3,n} &= (h/2)A_{n+\alpha} + (\gamma/2)h^2\dot{A}_{n+\beta} \\ &\quad + \delta h^3(\dot{A}_{n+\beta}A_{n+\alpha} - A_{n+\alpha}\dot{A}_{n+\beta}) \end{aligned} \tag{54d}$$

The coefficients α, β, γ, and δ will be determined later. From Propositions 5–7, we have

$$\Pi_{3,n} = kI \tag{55}$$

and $\Omega_{3,n}$ has the same form as S as shown in Eq. (10). By using Theorems 1 and 2, we conclude that the proposed third-order integrator is an A-stable constraint-preserving integrator. By expanding Eq. (54b), one obtains

$$J_{3,n} = I + hA_{n+\alpha} + (h^2/2)\left[A^2_{n+\alpha} + (\gamma/3)\dot{A}_{n+\beta}\right] + (h^3/6)A^3_{n+\alpha} + h^3[(\gamma/12 + 2\delta)\dot{A}_{n+\beta}A_{n+\alpha} + (\gamma/12 - 2\delta)A_{n+\alpha}\dot{A}_{n+\beta}] + O(h^4) \tag{56}$$

The matrices $A_{n+\alpha}$ and $\dot{A}_{n+\beta}$ in Eq. (56) are approximated by using the Taylor series

$$A_{n+\alpha} = A_n + \alpha h\dot{A}_n + (\alpha^2 h^2/2) + \ddot{A}_n + O(h^3) \tag{57a}$$

$$\dot{A}_{n+\beta} = \dot{A}_n + \beta h\ddot{A}_n + O(h^2) \tag{57b}$$

substituting Eqs. (57a) and (57b) into Eq. (56), we have

$$J_{3,n} = I + hA_n + h^2\left[\tfrac{1}{2}A^2_n + (\alpha + \gamma/6)\dot{A}_n\right] + h^3\left[\tfrac{1}{6}A^3_n + (\alpha^2/2 + \beta\gamma/6)\ddot{A}_n + (\alpha/2 + \gamma/12 + 2\delta)\dot{A}_nA_n + (\alpha/2 + \gamma/12 - 2\delta)A_n\dot{A}_n\right] + O(h^4) \tag{58}$$

By comparing the coefficients in Eq. (58) with the coefficients in Eq. (45), we have the equalities

$$\alpha + \gamma/6 = \tfrac{1}{2} \tag{59a}$$

$$\alpha^2/2 + \beta\gamma/6 = \tfrac{1}{6} \tag{59b}$$

$$\alpha/2 + \gamma/12 + 2\delta = \tfrac{1}{3} \tag{59c}$$

$$\alpha/2 + \gamma/12 - 2\delta = \tfrac{1}{6} \tag{59d}$$

and by manipulating the above equations, we have

$$\alpha + \gamma/6 = \tfrac{1}{2} \tag{60a}$$

$$\alpha^2/2 + \beta\gamma/6 = \tfrac{1}{6} \tag{60b}$$

$$\delta = \tfrac{1}{24} \tag{60c}$$

The solutions of Eqs. (60a–60c) are infinitely many. If we assume the integrator is equally spaced, the following quantities are obtained:

$$\alpha = \tfrac{1}{3}, \qquad \beta = \tfrac{2}{3}, \qquad \gamma = 1, \qquad \delta = \tfrac{1}{24} \tag{61}$$

d) Fourth-order integrator:

$$(\Pi_4 - \Omega_4)\boldsymbol{q}_{n+1} = (\Pi_4 + \Omega_4)\boldsymbol{q}_n \tag{62a}$$

or

$$\boldsymbol{q}_{n+1} = (\Pi_4 - \Omega_4)^{-1}(\Pi_4 + \Omega_4)\boldsymbol{q}_n \equiv J_{4,n}\boldsymbol{q}_n \tag{62b}$$

where

$$\Pi_4 = I + (h^2/12)A^2_{n+\frac{1}{2}} \tag{62c}$$

$$\Omega_4 = (h/2)A_{n+\frac{1}{2}} + (h^3/48)\left[\ddot{A}_{n+\frac{1}{2}} + 2\left(\dot{A}_{n+\frac{1}{2}}A_{n+\frac{1}{2}} - A_{n+\frac{1}{2}}\dot{A}_{n+\frac{1}{2}}\right)\right] \tag{62d}$$

From Proposition 5, we have

$$\Pi_{4,n} = kI \tag{63}$$

and $\Omega_{4,n}$ has the same form as shown in Eq. (10). Again, by using Theorems 1 and 2, we conclude that the proposed fourth-order integrator is an A-stable constraint-preserving integrator.

Accuracy analysis: By rewriting the matrix $J_{4,n}$ given in Eq. (62b), we get

$$J_{4,n} = I + hA_{n+\frac{1}{2}} + (h^2/2)A^2_{n+\frac{1}{2}} + h^3\left[\tfrac{1}{6}A^3_{n+\frac{1}{2}} + \tfrac{1}{24}\ddot{A}_{n+\frac{1}{2}} + \tfrac{1}{12}\left(\dot{A}_{n+\frac{1}{2}}A_{n+\frac{1}{2}} - A_{n+\frac{1}{2}}\dot{A}_{n+\frac{1}{2}}\right)\right] + (h^4/24)\left[A^4_{n+\frac{1}{2}} + \tfrac{1}{2}\left(\ddot{A}_{n+\frac{1}{2}}A_{n+\frac{1}{2}} + A_{n+\frac{1}{2}}\ddot{A}_{n+\frac{1}{2}}\right) + \dot{A}_{n+\frac{1}{2}}A^2_{n+\frac{1}{2}} - A^2_{n+\frac{1}{2}}\dot{A}_{n+\frac{1}{2}}\right] + O(h^5) \tag{64}$$

By approximating the matrices $A_{n+1/2}$, $\dot{A}_{n+1/2}$, and $\ddot{A}_{n+1/2}$ in Eq. (64) by the Taylor series, we obtain

$$A_{n+\frac{1}{2}} = A_n + (h/2)\dot{A}_n + (h^2/8)\ddot{A}_n + (h^3/48)\dddot{A}_n + O(h^4) \tag{65a}$$

$$\dot{A}_{n+\frac{1}{2}} = \ddot{A}_n + (h/2)\ddot{A}_n + (h^2/8)\dddot{A}_n + O(h^3) \tag{65b}$$

$$\ddot{A}_{n+\frac{1}{2}} = \ddot{A}_n + (h/2)\dddot{A}_n + O(h^2) \tag{65c}$$

Substituting Eqs. (65a–65c) into Eq. (64) yields

$$\boldsymbol{q}_{n+1} = \boldsymbol{q}_n + hA_n\boldsymbol{q}_n + (h^2/2)\left(A^2_n + \dot{A}_n\right) + (h^3/6)\left(A^3_n + \ddot{A}_n + 2\dot{A}_nA_n + A_n\dot{A}_n\right)\boldsymbol{q}_n + (h^4/24)\left(A^4_n + A^2_n\dot{A}_n + 2A_n\dot{A}_nA_n + A_n\ddot{A}_n + 3\dot{A}_nA^2_n + 3\dot{A}^2_n + 3\ddot{A}_nA_n + \dddot{A}_n\right)\boldsymbol{q}_n + O(h^5) \tag{66}$$

By comparing the coefficients involved in Eq. (66) with the coefficients in Eq. (45), we conclude that the integrator described in Eq. (62a–62d) is a fourth-order integrator.

Reducing the computational costs:

The proposed constraint-preserving integrators described in Eqs. (46a), (50a), (54a), and (62a) require us to solve a set of linear equations, and these processes are time-consuming. To overcome this difficulty, alternative computational algorithms based on Proposition 4 and Remark 1 are developed:

For the first-order integrator:

$$\boldsymbol{q}_{n+1} = (1/\Delta_{1,n})[I + (h/2)A_n]^2\boldsymbol{q}_n = J_{1,n}\boldsymbol{q}_n \tag{67a}$$

$$\Delta_{1,n} = 1 + (h^2/16)\left[\omega^2_1(t_n) + \omega^2_2(t_n) + \omega^2_3(t_n)\right] \tag{67b}$$

For the second-order integrator:

$$\boldsymbol{q}_{n+1} = (1/\Delta_{2,n})\left[I + (h/2)A_{n+\frac{1}{2}}\right]^2\boldsymbol{q}_n = J_{2,n}\boldsymbol{q}_n \tag{68a}$$

$$\Delta_{2,n} = 1 + (h^2/16)\left[\omega^2_1\left(t_{n+\frac{1}{2}}\right) + \omega^2_2\left(t_{n+\frac{1}{2}}\right) + \omega^2_3\left(t_{n+\frac{1}{2}}\right)\right] \tag{68b}$$

For the third-order integrator:

$$\boldsymbol{q}_{n+1} = (1/\Delta_{3,n})[\Pi_{3,n} + \Omega_{3,n}]^2\boldsymbol{q}_n = J_{3,n}\boldsymbol{q}_n \tag{69a}$$

$$\Pi_{3,n} = I + (h^2/12)A^2_{n+\frac{1}{3}} \tag{69b}$$

$$\Omega_{3,n} = (h/2)A_{n+\frac{1}{3}} + \tfrac{1}{3}h^2\dot{A}_{n+\frac{2}{3}} + \tfrac{1}{24}h^3\left(\dot{A}_{n+\frac{2}{3}}A_{n+\frac{1}{3}} - A_{n+\frac{1}{3}}\dot{A}_{n+\frac{2}{3}}\right) \tag{69c}$$

where $\Delta_{3,n}$ is the square of norm-2 of any column (row) involved in the matrix $[\Pi_{3,n} + \Omega_{3,n}]$.

For the fourth-order integrator:

$$q_{n+1} = (1/\Delta_{4,n})[\Pi_{4,n} + \Omega_{4,n}]^2 q_n = J_{4,n} q_n \tag{70a}$$

$$\Pi_{4,n} = I + (h^2/12) A^2_{n+\frac{1}{2}} \tag{70b}$$

$$\Omega_{4,n} = (h/2) A_{n+\frac{1}{2}} + (h^3/48)\Big[\ddot{A}_{n+\frac{1}{2}} + 2\Big(\dot{A}_{n+\frac{1}{2}} A_{n+\frac{1}{2}} - A_{n+\frac{1}{2}} \dot{A}_{n+\frac{1}{2}}\Big)\Big] \tag{70c}$$

where $\Delta_{4,n}$ is the square of norm-2 of any column (row) involved in the matrix $\lfloor \Pi_{4,n} + \Omega_{4,n} \rfloor$.

V. Numerical Example

In the present numerical example, we use two data sets given by Yen and Cook.[6]

Data set 1: $\omega_1 = 2\sin t$, $\omega_2 = \omega_1$, and $\omega_3 = 10\sin 0.5t$

Data set 2: $\omega_1 = 0.25\sin 12t$, $\omega_2 = 0.25\cos 12t$, and $\omega_3 = 5\sin 0.25t$

The initial conditions of Euler parameters are $q_0 = 1$ and $q_1 = q_2 = q_3 = 0$. For the present numerical simulation, we assume that the solutions of Euler parameters can be obtained using the fourth-order integrator with step size equal to 0.0001 s. By using three different step sizes for each set of data, we can compare the state error at specific time frames. On the one hand, as observed from Tables 1 and 2, the state errors of q_0 at $t = 10$ s increase while the step size increases. On the other hand, with the same time step, the state errors decrease while the order of the integrator increases. These results show that the accuracy of Euler parameters is highly dependent on the step sizes, the angular velocities, and the order of employed time integrators.

From the constraint-preserving aspect of the problem, Figs. 1 and 2 have illustrated that regardless of the choice of order of the integrator, the constraint errors remain within 10^{-14} (about the machine constant) for the two different data sets. As shown in Fig. 3, the constraint errors of data set 2 remain within 10^{-15} for step sizes varying from 0.01 to 1. These results show that the constraint errors will not be affected by the chosen time steps. As observed from Fig. 3, the value $h = 1$ experiences the smallest constraint error. The reason is that during the 100-s numerical simulation, $h = 1$ requires only 100 time steps in comparison to $h = 0.01$, which requires 10,000 time steps. By increasing the number of time steps, the calculations of transform matrix J are simultaneously increased; this procedure will compound the constraint errors over the time span. However, as illustrated in Fig. 3, the constraint errors are oscillating between $\pm 10^{-14}$ for the chosen time steps. In conclusion, from Figs. 1 to 3, we have successfully demonstrated our claim in Theorem 1.

Table 1 Errors of q_0 for data set 1 at t = 10 s

Order	Value of h: 0.1	0.01	0.001
1st	$-1.4080E-1$	$-2.2572E-2$	$-2.3372E-3$
2nd	$8.6890E-2$	$9.0145E-4$	$9.0177E-6$
3rd	$-7.7376E-4$	$-1.0004E-6$	$-1.0224E-9$
4th	$2.3684E-4$	$2.3965E-8$	$1.4157E-12$

Table 2 Errors of q_0 for data set 2 at t = 10 s

Order	Value of h: 0.1	0.01	0.001
1st	$-1.1225E-1$	$6.1765E-3$	$-5.7061E-4$
2nd	$-4.9979E-2$	$-4.9033E-4$	$-4.9023E-6$
3rd	$6.1290E-5$	$-1.4787E-8$	$-3.9696E-11$
4th	$-1.1021E-4$	$-1.1143E-8$	$3.4505E-13$

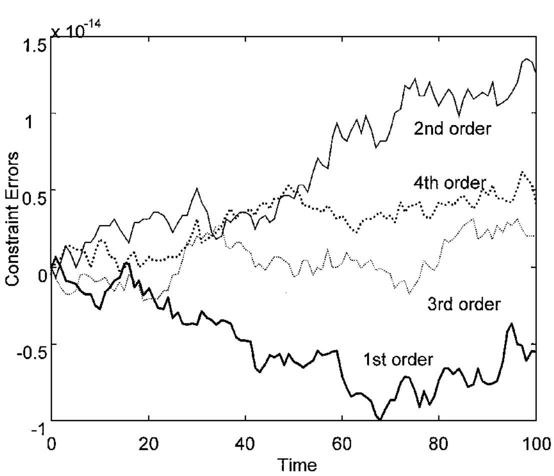

Fig. 1 Constraint errors for data set 1 (h = 0.1).

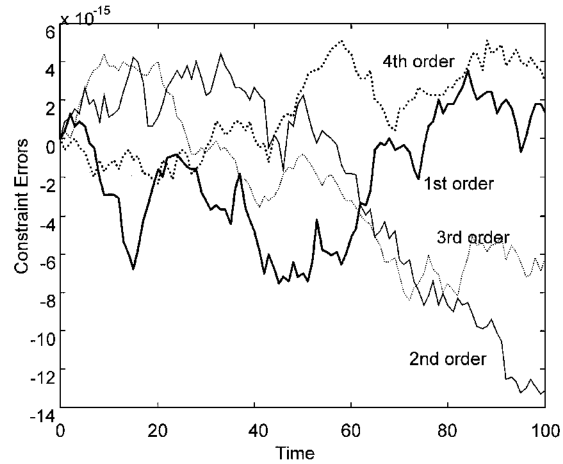

Fig. 2 Constraint errors for data set 2 (h = 0.1).

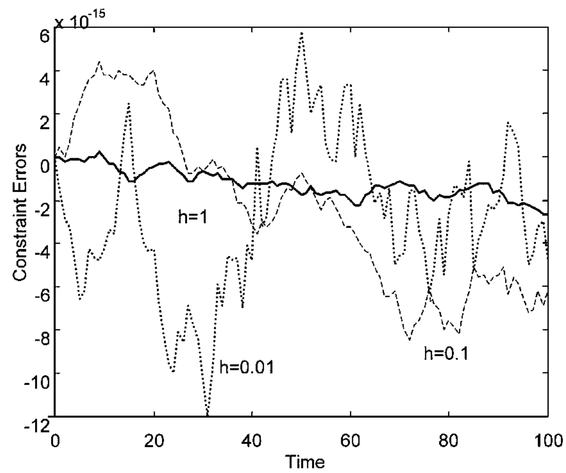

Fig. 3 Constraint errors for data set 2 (third-order integrator with three different step sizes).

VI. Conclusions

In this paper, the generalized constraint-preserving integrators for solving quaternion equations are derived. The integrators proposed by Park and Chiou are shown to be second-order constraint-preserving integrators. To improve the accuracy of the Park–Chiou integrator, the third- and fourth-order constraint-preserving integrators used in solving the quaternion equations are also given. Note that the proposed fourth-order integrator needs to compute the second time derivative of the angular velocity $\ddot{\omega}_i$ ($i = 1, 2, 3$). For the kinematic analysis, $\ddot{\omega}_i$ ($i = 1, 2, 3$) can be directly differentiated from the given data sets as shown in the numerical examples. However, for dynamic analysis, the computational cost of the proposed algorithm is very high. The algorithms that overcome this difficulty are still under investigation, and we hope to report this effort in the near future.

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References

[1]Wittenburg, J., "A New Correction Formula for Euler–Rodrigues Parameters," *ZAMM*, Vol. 62, 1982, pp. 495–497.

[2]Conte, S. D., and de Boor, C., *Elementary Numerical Analysis*, McGraw–Hill, New York, 1965.

[3]Gerald, C. F., *Applied Numerical Analysis*, Addison Wesley Longman, Reading, MA, 1978.

[4]Wilson, J. W., and Steinmetz, G. G., "Analysis of Numerical Integration Techniques for Real-Time Digital Flight Simulation," NASA TN D-4900, 1968.

[5]Lawrence, E. B., Jr., Bowles, R. L., and Williams, L. H., "Development and Application of a Local Linearization Algorithm for the Integration of Quaternion Rate Equations in Real-Time Flight Simulation Problems," NASA TN D-7347, 1973.

[6]Yen, K., and Cook, G., "Improved Local Linearization Algorithm for Solving the Quaternion Equations," *Journal of Guidance and Control*, Vol. 3, No. 5, 1980, pp. 468–471.

[7]Nikravesh, P. E., *Computer-Aided Analysis of Mechanical System*, Prentice–Hall, Englewood Cliffs, NJ, 1988, pp. 315, 316.

[8]Abia, L., and Sanz-Serna, J. M., "Partitioned Runge–Kutta Methods for Separable Hamiltonian Problem," *Mathematics of Computation*, Vol. 60, No. 202, 1993, pp. 617–634.

[9]Jay, L., "Symplectic Partitioned Runge–Kutta Methods for Constrained Hamiltonian Systems," *SIAM Journal on Numerical Analysis*, Vol. 33, No. 1, 1996, pp. 368–397.

[10]Okunbor, D. I., "Energy Conserving, Liouville, and Symplectic Integrators," *Journal of Computational Physics*, Vol. 120, 1995, pp. 375–378.

[11]Senz-Serna, J. M., and Portillo, A., "Classical Numerical Integrator for Wave-Packet Dynamics," *Journal of Chemical Physics*, Vol. 104, No. 6, 1996, pp. 2349–2355.

[12]Yoshida, H., "Construction of Higher Order Symplectic Integrators," *Physics Letters A*, Vol. 150, Nos. 5–7, 1990, pp. 262–268.

[13]Chiou, J. C., "Constraint Treatment Techniques and Parallel Algorithms for Multibody Dynamic Analysis," Ph.D. Dissertation, Univ. of Colorado, Boulder, CO, 1990.

[14]Park, K. C., and Chiou, J. C., "A Discrete Momentum-Conserving Explicit Algorithm for Rigid Body Dynamics Analysis," *International Journal for Numerical Methods in Engineering*, Vol. 36, 1993, pp. 1071–1073.