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Math 189

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Final Project : "Unconditionally Stable Algorithms for Rigid Body Dynamics that Exactly Preserve Energy and Momentum", by J.C. Simo and K.K. Wong.

PART 1: The Rotation Group and Rigid Body Dynamics.

Let $\mathcal{B} \subset \mathbb{R}^3$ be the reference placement of a solid body, with material particles labelled by $\underset{\sim}{X}$. A motion of the body is a one paramter family of mappings

$$\underset{\sim}{\Phi}_t : \mathcal{B} \longrightarrow \mathbb{R}^3 , \quad \text{for } t \in [0,T] \subset \mathbb{R}_+ .$$

The motion is rigid if

$$\| \underset{\sim}{\Phi}_t(\underset{\sim}{X}_1) - \underset{\sim}{\Phi}_t(\underset{\sim}{X}_2) \| = \| \underset{\sim}{X}_1 - \underset{\sim}{X}_2 \| \quad \forall \underset{\sim}{X}_1, \underset{\sim}{X}_2 \in \mathcal{B} \text{ and } t \in [0,T].$$

This condition holds if and only if $\underset{\sim}{\Phi}_t$ is of the form

$$\underset{\sim}{x} = \underset{\sim}{\Phi}_t := \underset{\sim}{\varphi}(t) + \underset{\sim}{\Lambda}(t)\underset{\sim}{X}$$

where $\underset{\sim}{\Lambda}(t) \in SO(3)$, the special orthogonal group, $\forall t \in [0,T]$ and $t \longmapsto \underset{\sim}{\varphi}(t)$ is a time dependent vector-valued function. Thus, any mapping

$$t \in [0,T] \longmapsto (\underset{\sim}{\varphi}(t), \underset{\sim}{\Lambda}(t)) \in \mathbb{R}^3 \times SO(3)$$

defines a rigid motion of the body. We thus refer to $Q := \mathbb{R}^3 \times SO(3)$ as the abstract configuration manifold of the rigid body.

Let $\rho_0 : \mathcal{B} \longrightarrow \mathbb{R}$ be the reference density of the body in the placement $\mathcal{B}$. Choose coordinates in $\mathcal{B}$ so that the center of mass is at the origin. We then have

$$\int_{\mathcal{B}} \rho_0 \underset{\sim}{X} \, d\underset{\sim}{X} = \underset{\sim}{0} .$$

Let $\{\underset{\sim}{E}_1, \underset{\sim}{E}_2, \underset{\sim}{E}_3\}$ denote the basis vectors for the reference frame $\mathcal{B}$. Let $\{\underset{\sim}{e}_1, \underset{\sim}{e}_2, \underset{\sim}{e}_3\}$ denote the basis vectors for the current configuration $\underset{\sim}{\Phi}_t(\mathcal{B})$. We refer to $\{\underset{\sim}{e}_1, \underset{\sim}{e}_2, \underset{\sim}{e}_3\}$ as the inertial frame. We shall assume $\underset{\sim}{e}_i = \underset{\sim}{E}_i$ for convenience.

By our choice of coordinate systems, the map $t \longmapsto \underset{\sim}{\varphi}(t)$ defines the center of mass at time t (we assume $\underset{\sim}{\varphi}(t)|_{t=0} = \underset{\sim}{0}$). Additionally, the map $t \to \underset{\sim}{\Lambda}(t)$ defines the orientation of the frame $\{\underset{\sim}{E}_1, \underset{\sim}{E}_2, \underset{\sim}{E}_3\}$ according to the relationship

$$\underset{\sim}{t}_A(t) := \underset{\sim}{\Lambda}(t)\underset{\sim}{E}_A , \quad A = 1,2,3 .$$

We call $\{\underset{\sim}{t}_A(t)\}_{A=1,2,3}$, with $\underset{\sim}{t}_A(0) = \underset{\sim}{E}_A$, the body frame. We also have the relationship

$$\underset{\sim}{\Lambda}(t) = \underset{\sim}{t}_A(t) \otimes \underset{\sim}{E}_A$$

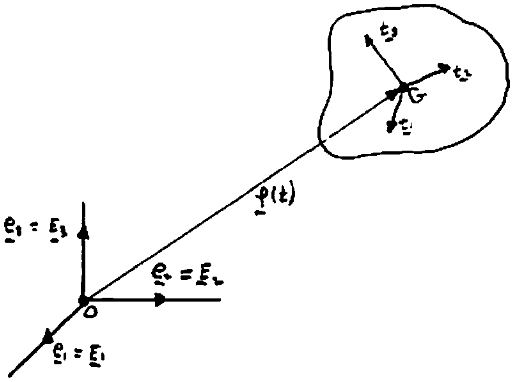

Figure : Kinematics of the Rigid Body.

For the rigid body motion, the velocity field is given by

$$\dot{x} = \dot{\Phi}_t = \dot{\varphi}(t) + \dot{\Lambda}(t)\, X, \quad (X, t) \in \mathcal{B} \times [0, T].$$

In this case, $\dot{\varphi}(t)$ is the translational velocity of the center of mass. Since $\Lambda(t) \in SO(3)$ $\forall\, t \in [0, T]$ we have $\Lambda(t)\Lambda^T(t) = \Lambda^T(t)\Lambda(t) = I$ and we can write

$$\dot{\Lambda}(t) = \dot{\Lambda}(t)\Lambda^T(t)\Lambda(t) = \Lambda(t)\Lambda^T(t)\dot{\Lambda}(t).$$

$$\dot{\Lambda}(t) = \hat{w}(t)\Lambda(t) = \Lambda(t)\hat{W}(t)$$

where $\hat{w}(t) = \dot{\Lambda}(t)\Lambda^T(t)$ and $\hat{W} = \Lambda^T(t)\dot{\Lambda}(t)$.

Lemma 1: $\hat{w}$ and $\hat{W}$ are skew symmetric.

Proof : $\Lambda\Lambda^T = I$. Then, $\dot{\Lambda}\Lambda^T + \Lambda\dot{\Lambda}^T = 0$. So $\dot{\Lambda}\Lambda^T = -\Lambda\dot{\Lambda}^T$

$$\hat{w}^T = (\dot{\Lambda}\Lambda^T)^T = \Lambda\dot{\Lambda}^T = -\dot{\Lambda}\Lambda^T = -\hat{w} \checkmark$$

$\Lambda^T\Lambda = I$. Then, $\dot{\Lambda}^T\Lambda + \Lambda^T\dot{\Lambda} = 0$. So $\dot{\Lambda}^T\Lambda = -\Lambda^T\dot{\Lambda}$

$$\hat{W}^T = (\Lambda^T\dot{\Lambda})^T = \dot{\Lambda}^T\Lambda = -\Lambda^T\dot{\Lambda} = -\hat{W} \checkmark$$

$\boxtimes$

Denote by $so(3)$ the vector space of skew-symmetric matrices.
$so(3) = \{ \hat{w} : \mathbb{R}^3 \to \mathbb{R}^3 \mid \text{linear and } \hat{w} + \hat{w}^T = 0 \}$.

Define the hat map $\wedge : \mathbb{R}^3 \to so(3)$ by

$$\{w\} = \begin{Bmatrix} w_1 \\ w_2 \\ w_3 \end{Bmatrix} \in \mathbb{R}^3 \longmapsto [\hat{w}] = \begin{bmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{bmatrix} \in so(3).$$

We refer to w as the axial vector associated with $\hat{w}$.

Define the wedge map $^\vee : so(3) \to \mathbb{R}^3$ as the inverse of the hap map $^\wedge$. $\hat{\underset{\sim}{W}}$ and its' associated axial vector are also related by

$$\hat{\underset{\sim}{W}} \underset{\sim}{h} = \underset{\sim}{W} \times \underset{\sim}{h} \quad \forall \ \underset{\sim}{h} \in \mathbb{R}^3$$

where $\times$ is the ordinary cross product on $\mathbb{R}^3$. The axial vectors $\underset{\sim}{w}(t)$ and $\underset{\sim}{W}(t)$ associated with $\hat{\underset{\sim}{w}}(t)$ and $\hat{\underset{\sim}{W}}(t)$ are referred to as spatial and convected angular velocities, respectively.

Lemma 2: The spatial angular velocity $\underset{\sim}{w}$ is the angular velocity of the body frame.

Proof: $\dot{\underset{\sim}{t}}_A = \dot{\underset{\sim}{\Lambda}} \underset{\sim}{E}_A = \dot{\underset{\sim}{\Lambda}} \underset{\sim}{\Lambda}^T \underset{\sim}{t}_A = \hat{\underset{\sim}{w}} \underset{\sim}{t}_A = \underset{\sim}{w} \times \underset{\sim}{t}_A$. $\boxed{}$

Lemma 3: $\hat{\underset{\sim}{w}} = \underset{\sim}{\Lambda} \hat{\underset{\sim}{W}} \underset{\sim}{\Lambda}^T$ and $\underset{\sim}{w} = \underset{\sim}{\Lambda} \underset{\sim}{W}$.

Proof: $\hat{\underset{\sim}{w}} = \dot{\underset{\sim}{\Lambda}} \underset{\sim}{\Lambda}^T = \underset{\sim}{\Lambda} \hat{\underset{\sim}{W}} \underset{\sim}{\Lambda}^T$ ✓

Since $\hat{w} h = w \times h$, we know $\hat{\underset{\sim}{w}} \underset{\sim}{w} = \underset{\sim}{w} \times \underset{\sim}{w} = \underset{\sim}{0}$.
Then,

$$\underset{\sim}{\Lambda} \hat{\underset{\sim}{W}} \underset{\sim}{\Lambda}^T \underset{\sim}{w} = \underset{\sim}{0}$$

$$\hat{\underset{\sim}{W}} \underset{\sim}{\Lambda}^T \underset{\sim}{w} = \underset{\sim}{0}$$

$$\underset{\sim}{W} \times \underset{\sim}{\Lambda}^T \underset{\sim}{w} = \underset{\sim}{0}.$$

So $\underset{\sim}{W} = \alpha \underset{\sim}{\Lambda}^T \underset{\sim}{w}$ for some $\alpha \in \mathbb{R}$.

$$
\begin{aligned}
\text{Now, } \underset{\sim}{W} \cdot \underset{\sim}{W} &= \tfrac{1}{2} \operatorname{tr} (\hat{\underset{\sim}{W}}^T \hat{\underset{\sim}{W}}) \\
&= \tfrac{1}{2} \operatorname{tr} (\underset{\sim}{\Lambda}^T \hat{\underset{\sim}{w}}^T \underset{\sim}{\Lambda} \underset{\sim}{\Lambda}^T \hat{\underset{\sim}{w}} \underset{\sim}{\Lambda}) \\
&= \tfrac{1}{2} \operatorname{tr} (\underset{\sim}{\Lambda}^T \hat{\underset{\sim}{w}}^T \hat{\underset{\sim}{w}} \underset{\sim}{\Lambda}) \\
&= 1/2 \, (\underset{\sim}{\Lambda}^T)_{Ai} (\hat{w}^T)_{ij} \hat{w}_{jk} \Lambda_{kA} \\
&= 1/2 \, \Lambda_{iA} \hat{w}_{ji} \hat{w}_{jk} \Lambda_{kA} \\
&= 1/2 \, \hat{w}_{ji} \hat{w}_{ji} \\
&= 1/2 \operatorname{tr} (\hat{\underset{\sim}{w}}^T \hat{\underset{\sim}{w}}) = \underset{\sim}{w} \cdot \underset{\sim}{w}.
\end{aligned}
$$

This means $\underset{\sim}{W} \cdot \underset{\sim}{W} = \alpha^2 \underset{\sim}{\Lambda}^T \underset{\sim}{w} \cdot \underset{\sim}{\Lambda}^T \underset{\sim}{w} = \alpha^2 \underset{\sim}{w} \cdot \underset{\sim}{w}$.

So $\alpha = \pm 1$. But when $\underset{\sim}{\Lambda} = \underset{\sim}{I}$, $\hat{\underset{\sim}{w}} = \hat{\underset{\sim}{W}}$ which implies that $\underset{\sim}{w} = \underset{\sim}{W}$ by the wedge map Thus, $\alpha = +1$. ✓

$\boxed{}$

Lemma 4: The components of the spatial angular velocity relative to the body frame equal the components of the convected angular velocity relative to the reference frame $\{E_1, E_2, E_3\}$.

Proof: $t_A \cdot w = \Lambda E_A \cdot w = E_A \cdot \Lambda^T w = E_A \cdot W$

Then, $w = (t_A \cdot w) t_A = (E_A \cdot W) t_A = W_A t_A$ $\blacksquare$

Denote by $J(t)$ the total angular momentum of the body. We define $J(t)$ with the following expression:

$$J(t) := \int_{\mathcal{B}} \rho_0 \, \phi_t(X) \times \dot{\phi}_t(X) \, dX .$$

Theorem 1: For the rigid body, $J(t) = \varphi(t) \times p(t) + \pi(t)$, where

$p(t) = M \dot{\varphi}(t)$, $M = \int_{\mathcal{B}} \rho_0 \, dX$, $\pi(t) = \Lambda(t) \mathbb{I} \Lambda^T(t) w(t)$

and $\mathbb{I} = \int_{\mathcal{B}} \rho_0 [\, \|X\|^2 I - X \otimes X \,] \, dX$.

Proof: For the rigid body,

$$J(t) = \int_{\mathcal{B}} \rho_0 \varphi(t) \times [\dot{\varphi}(t) + \dot{\Lambda}(t) X] \, dX$$
$$+ \int_{\mathcal{B}} \rho_0 \Lambda(t) X \times [\dot{\varphi}(t) + \dot{\Lambda}(t) X] \, dX .$$

Using the fact that $\int_{\mathcal{B}} \rho_0 X \, dX = 0$ by our choice of coordinate systems, we may reduce the above result to

$$J(t) = \int_{\mathcal{B}} \rho_0 \varphi(t) \times \dot{\varphi}(t) \, dX + \int_{\mathcal{B}} \rho_0 \Lambda(t) X \times \dot{\Lambda}(t) X \, dX$$

$$= \varphi(t) \times \dot{\varphi}(t) \int_{\mathcal{B}} \rho_0 \, dX + \int_{\mathcal{B}} \rho_0 \Lambda X \times \Lambda \hat{W} X \, dX$$

$$= \varphi(t) \times M \dot{\varphi}(t) + \int_{\mathcal{B}} \rho_0 \Lambda X \times [\Lambda (W \times X)] \, dX$$

$$= \varphi(t) \times p(t) + \int_{\mathcal{B}} \rho_0 \Lambda X \times [\Lambda (W \times X)] \, dX .$$

Let $\pi(t) = J(t) - \varphi(t) \times p(t)$.

Then, we have the expression

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$$\mathbf{S}(t) = \int_{\mathcal{B}} \rho_0 \Lambda \mathbf{X} \times [\Lambda(\mathbf{W} \times \mathbf{X})]\, d\mathbf{X}.$$

Choose $\mathbf{y} \in \mathbb{R}^3$. We now write

$$\Lambda \mathbf{y} \cdot \mathbf{S}(t) = \int_{\mathcal{B}} \rho_0 \Lambda \mathbf{y} \cdot [\Lambda \mathbf{X} \times \Lambda(\mathbf{W} \times \mathbf{X})]\, d\mathbf{X}$$

Making use of the identity $(\det \Lambda)[\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})] = [\Lambda \mathbf{a} \cdot (\Lambda \mathbf{b} \times \Lambda \mathbf{c})]$ and the fact that $\det \Lambda = 1$,

$$\Lambda \mathbf{y} \cdot \mathbf{S}(t) = \int_{\mathcal{B}} \rho_0 \mathbf{y} \cdot [\mathbf{X} \times (\mathbf{W} \times \mathbf{X})]\, d\mathbf{X}$$

$$\mathbf{y} \cdot \Lambda^T \mathbf{S}(t) = \mathbf{y} \cdot \int_{\mathcal{B}} \rho_0 [\mathbf{X} \times (\mathbf{W} \times \mathbf{X})]\, d\mathbf{X}$$

$$\Lambda^T \mathbf{S}(t) = \int_{\mathcal{B}} \rho_0 [\mathbf{X} \times (\mathbf{W} \times \mathbf{X})]\, d\mathbf{X}$$

Now, we have the identity $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c}$

$$\Lambda^T \mathbf{S}(t) = \int_{\mathcal{B}} \rho_0 [(\mathbf{X} \cdot \mathbf{X})\mathbf{W} - (\mathbf{X} \cdot \mathbf{W})\mathbf{X}]\, d\mathbf{X}$$

$$\Lambda^T \mathbf{S}(t) = \int_{\mathcal{B}} \rho_0 [\|\mathbf{X}\|^2 - \mathbf{X} \otimes \mathbf{X}]\, d\mathbf{X}\, \mathbf{W}$$

$$\mathbf{S}(t) = \Lambda \int_{\mathcal{B}} \rho_0 [\|\mathbf{X}\|^2 - \mathbf{X} \otimes \mathbf{X}]\, d\mathbf{X}\, \Lambda^T \mathbf{w}$$

Finally, this yields

$$\mathbf{J}(t) - \mathbf{f}(t) \times \mathbf{p}(t) = \Lambda(t)\, \mathbb{I}\, \Lambda^T(t)\, \mathbf{w}(t)$$

$$\mathbf{J} = \mathbf{f} \times \mathbf{p} + \boldsymbol{\pi}.$$

$\boxtimes$

M is the total mass of the body, and $\mathbf{p}(t)$ is the total linear momentum, $\boldsymbol{\pi}(t)$ is the total spatial angular momentum relative to the center of mass and $\mathbb{I}$ is the constant convected inertia tensor (or inertia dyadic).

Define the convected angular momentum relative to the center of mass by

$$\boldsymbol{\Pi}(t) = \Lambda^T(t)\, \boldsymbol{\pi}(t) = \mathbb{I}\mathbf{W}.$$

Let $\bar{m}(t)$ be the applied torque and let $\bar{n}(t)$ be the applied force at the center of mass. The classical equations of balance of angular and linear momentum are

$$\frac{d\pi}{dt} = \dot{\pi} = \bar{m} \;, \qquad \frac{dp}{dt} = \dot{p} = \bar{n} .$$

Let $a = \dot{w}$ and let $A = \dot{W}$. Then,

$$a = \frac{d}{dt}[\Lambda W] = \dot{\Lambda} W + \Lambda \dot{W} = \Lambda \cancel{\hat{W} W}^{\,0} + \Lambda \dot{W} = \Lambda A .$$

Now, we may express the balance of angular momentum equation in alternative ways.

$$\dot{\pi} = \bar{m}$$

$$\overline{(\Lambda \mathbb{J} W)}^{\boldsymbol{\cdot}} = \bar{m}$$

$$\dot{\Lambda} \mathbb{J} W + \Lambda \mathbb{J} \dot{W} = \bar{m}.$$

$$\Lambda \hat{W} \mathbb{J} W + \Lambda \mathbb{J} A = \bar{m}$$

Then, $W \times \mathbb{J} W + \mathbb{J} A = \Lambda^T \bar{m}$.

$$\dot{\Lambda} \mathbb{J} W + \Lambda \mathbb{J} \dot{W} = \bar{m}.$$

$$\hat{w} \Lambda \mathbb{J} \Lambda^T w + \Lambda \mathbb{J} \Lambda^T a = \bar{m} .$$

Then, $w \times (\Lambda \mathbb{J} \Lambda^T) w + (\Lambda \mathbb{J} \Lambda^T) a = \bar{m}$.

We now have two (2) alternative formulations for the angular motion of a rigid body.

Convected (Reference)	Spatial
$\dot{\Lambda} = \Lambda \hat{W}$	$\dot{\Lambda} = \hat{w} \Lambda$
$\dot{W} = A$	$\dot{w} = a$
$\mathbb{J} A + W \times \mathbb{J} W = \Lambda^T \bar{m}$.	$(\Lambda \mathbb{J} \Lambda^T) a + w \times (\Lambda \mathbb{J} \Lambda^T) w = \bar{m}$.

We observe that we may pass from the convected representation to the spatial representation by transforming $(W, A) \longmapsto (w, a)$.

In subsequent developments, we shall assume $\bar{n} = 0$ so that the center of mass moves with constant linear velocity. We shall concern ourselves with only the rotational dynamics. The configuration manifold is simply $\mathcal{Q} = SO(3)$.

PART 2: The Exponential Map. Optimal Parameterizations.

One views the rotation group as a "curved surface" whose points, $\underset{\sim}{\Lambda} \in SO(3)$, represent finite rotations. An infinitesimal rotation is a skew-symmetric matrix $\hat{\underset{\sim}{\theta}} \in so(3)$ with associated axial vector $\underset{\sim}{\theta} \in \mathbb{R}^3$, which is interpreted as defining at tangent vector the surface $SO(3)$.
More concretely,

$$so(3) = T_{\underset{\sim}{I}} SO(3).$$

Consider a one-parameter family of infinitesimal rotations $\varepsilon \longmapsto \varepsilon \hat{\underset{\sim}{\theta}} \in so(3)$ interpreted geometrically as a line tangent to $SO(3)$. This straight line is tangent at the identity $\underset{\sim}{I}$ to the curve $\varepsilon \longmapsto \underset{\sim}{\Lambda}_\varepsilon \in SO(3)$, which is defined by the exponential map as

$$\varepsilon \in \mathbb{R} \longmapsto \underset{\sim}{\Lambda}_\varepsilon = \exp[\varepsilon \hat{\underset{\sim}{\theta}}] = \sum_{n=1}^{\infty} \frac{1}{n!}[\varepsilon \hat{\underset{\sim}{\theta}}]^n \in SO(3).$$

This series has a closed form expression

$$\underset{\sim}{\Lambda} = \exp[\hat{\underset{\sim}{\theta}}] = \underset{\sim}{I} + \frac{\sin\|\underset{\sim}{\theta}\|}{\|\underset{\sim}{\theta}\|} \hat{\underset{\sim}{\theta}} + \frac{1}{2} \frac{\sin^2 \|\underset{\sim}{\theta}\|}{[\frac{1}{2}\|\underset{\sim}{\theta}\|]^2} \hat{\underset{\sim}{\theta}}^2 .$$

By setting $\varepsilon = 1$, we define the proper orthogonal matrix $\underset{\sim}{\Lambda} = \exp[\hat{\underset{\sim}{\theta}}]$ associated with a given skew-symmetric matrix $\hat{\underset{\sim}{\theta}} \in so(3)$. Additionally, since $\hat{\underset{\sim}{\theta}}\underset{\sim}{\theta} = 0$, we see that $\exp[\hat{\underset{\sim}{\theta}}]\underset{\sim}{\theta} = \underset{\sim}{I}$. Thus, $\underset{\sim}{\theta}$ is an eigenvector of $\exp[\hat{\underset{\sim}{\theta}}]$ with eigenvalue 1. We interpret $\exp[\hat{\underset{\sim}{\theta}}]$ as a finite rotation, with rotation vector $\theta \in \mathbb{R}^3$ and rotation angle $\|\underset{\sim}{\theta}\|$.

The optimal singularity-free parameterization of $SO(3)$ is defined in terms of the four unit quaternion parameters, denoted by $(q_0, \underset{\sim}{q})$. Unit quaternion parameters are elements of the 3-sphere $S^3 \subset \mathbb{R}^4$. Thus, $q_0^2 + \underset{\sim}{q}\cdot\underset{\sim}{q} = 1$. The parameterization $(q_0, \underset{\sim}{q}) \longmapsto \underset{\sim}{\Lambda} \in SO(3)$ is defined by the standard formula

$$\underset{\sim}{\Lambda} = (2q_0^2 - 1)\underset{\sim}{I} + 2q_0 \hat{\underset{\sim}{q}} + 2\underset{\sim}{q} \otimes \underset{\sim}{q} .$$

The inverse parameterization $\underset{\sim}{\Lambda} \in SO(3) \longmapsto (q_0, \underset{\sim}{q}) \in S^3$ is defined by

$$q_0 = \frac{1}{2}\sqrt{1 + \mathrm{tr}\underset{\sim}{\Lambda}} \; ; \quad \underset{\sim}{q} = \frac{1}{4q_0} \widecheck{(\underset{\sim}{\Lambda} - \underset{\sim}{\Lambda}^T)} .$$

Given quaternion parameters $(p_0, \underset{\sim}{p})$, $(q_0, \underset{\sim}{q})$, $(r_0, \underset{\sim}{r})$ associated with $\underset{\sim}{P}, \underset{\sim}{Q}, \underset{\sim}{R} \in SO(3)$, matrix multiplication and quaternion multiplication are in one-to-one correspondence

$$\underset{\sim}{R} = \underset{\sim}{P}\underset{\sim}{Q} \longleftrightarrow (r_0, \underset{\sim}{r}) = (p_0, \underset{\sim}{p}) \circ (q_0, \underset{\sim}{q})$$

$$r_0 := p_0 q_0 - \underset{\sim}{p}\cdot\underset{\sim}{q}$$

$$\underset{\sim}{r} := p_0 \underset{\sim}{q} + q_0 \underset{\sim}{p} + \underset{\sim}{p} \times \underset{\sim}{q} .$$

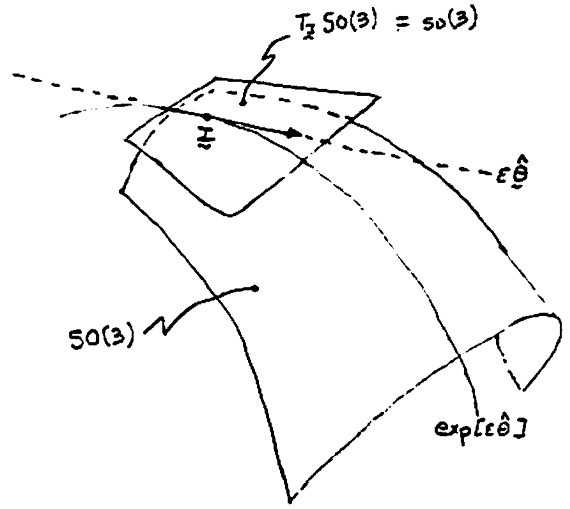

Figure : Graphical Interpretation of SO(3), so(3) and $\exp[\hat{\underset{\sim}{\theta}}]$.

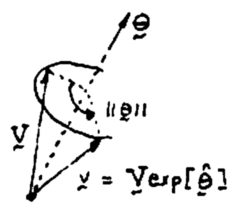

Figure : Interpretation of $\exp[\hat{\underset{\sim}{\theta}}]$ in terms of a rotation through angle $\|\underset{\sim}{\theta}\|$.

PART 3 : A Generalized Newmark Algorithm for SO(3).

Let $[t_n, t_{n+1}] \subseteq [0,T]$ be a typical time interval, where

$$[0,T] = \bigcup_{n=1}^{N} [t_n, t_{n+1}] .$$

Let $h = t_{n+1} - t_n$ be the time step interval. Assume that at t_n the following initial data are known :

$$(\underset{\sim}{\Lambda}_n, \underset{\sim}{W}_n, \underset{\sim}{A}_n) \in SO(3) \times \mathbb{R}^3 \times \mathbb{R}^3 .$$

Our objective is to obtain an algorithmic approximation

$$(\underset{\sim}{\Lambda}_{n+1}, \underset{\sim}{W}_{n+1}, \underset{\sim}{A}_{n+1}) \in SO(3) \times \mathbb{R}^3 \times \mathbb{R}^3$$

to the actual solution $(\underset{\sim}{\Lambda}(t_{n+1}), \underset{\sim}{W}(t_{n+1}), \underset{\sim}{A}(t_{n+1}))$ of the evolution equations governing the rotational dynamics of the rigid body. We shall use the convective representation of the motion in our algorithm.

Consider the following algorithm ALGO-1 :

Step 1. Define the updated configuration via the exponential map as

$$\underset{\sim}{\Lambda}_{n+1} = \underset{\sim}{\Lambda}_n \exp[\hat{\underset{\sim}{\Theta}}]$$

where $\underset{\sim}{\Theta} \in \mathbb{R}^3$ is the convected relative incremental rotation vector.

Step 2. Define $\underset{\sim}{\Theta} \in \mathbb{R}^3$ in terms of $(\underset{\sim}{W}_n, \underset{\sim}{A}_n, \underset{\sim}{A}_{n+1})$ by the formula

$$\underset{\sim}{\Theta} = h \underset{\sim}{W}_n + h^2 [(1/2 - \beta) \underset{\sim}{A}_n + \beta \underset{\sim}{A}_{n+1}]$$

where $\beta \in [0, 1/2]$ is a parameter with identical significance as in the classical Newmark algorithm.

Step 3. Define the updated convected angular velocity $\underset{\sim}{W}_{n+1}$ by the formula

$$\underset{\sim}{W}_{n+1} = \underset{\sim}{W}_n + h[(1-\gamma)\underset{\sim}{A}_n + \gamma \underset{\sim}{A}_{n+1}]$$

where $\gamma \in [0,1]$ is a parameter with identical significance as in the classical Newmark algorithm.

Step 4. Enforce <u>rate</u> of momentum balance at $t_n + \gamma h$

$$\underset{\sim}{J} \underset{\sim}{A}_{n+\gamma} + \underset{\sim}{W}_{n+\gamma} \times \underset{\sim}{J} \underset{\sim}{W}_{n+\gamma} = \underset{\sim}{\Lambda}^T_{n+\gamma} \underset{\sim}{\bar{m}}_{n+\gamma}$$

where

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$$\underset{\sim}{A}_{n+\gamma} = (1-\gamma)\underset{\sim}{A}_n + \gamma\underset{\sim}{A}_{n+1} .$$

$$\underset{\sim}{W}_{n+\gamma} = (1-\gamma)\underset{\sim}{W}_n + \gamma\underset{\sim}{W}_{n+1} .$$

$$\overline{\underset{\sim}{m}}_{n+\gamma} = (1-\gamma)\overline{m}_n + \gamma\overline{m}_{n+1} .$$

$$\underset{\sim}{\Lambda}_{n+\gamma} = \underset{\sim}{\Lambda}_n \exp[\gamma\hat{\underset{\sim}{\theta}}].$$

Theorem 2 : Let the applied torque in the interval $[t_n, t_{n+1}]$ be zero. Then, the total energy and the norm of the angular momentum are conserved by ALGO-I if and only if $\gamma = 1/2$, regardless of the choice of the paramter β.

Proof : We have angular velocity update formula

$$\underset{\sim}{W}_{n+1} = \underset{\sim}{W}_n + h[(1-\gamma)\underset{\sim}{A}_n + \gamma\underset{\sim}{A}_{n+1}]$$

$$\underset{\sim}{W}_{n+1} = \underset{\sim}{W}_n + h\underset{\sim}{A}_{n+\gamma}$$

Then, $\underset{\sim}{A}_{n+\gamma} = \frac{1}{h}(\underset{\sim}{W}_{n+1} - \underset{\sim}{W}_n)$.

We have the rate of momentum balance equation

$$\underset{\sim}{\mathbb{J}}\underset{\sim}{A}_{n+\gamma} + \underset{\sim}{W}_{n+\gamma} \times \underset{\sim}{\mathbb{J}}\underset{\sim}{W}_{n+\gamma} = \underset{\sim}{0}.$$

$$\underset{\sim}{\mathbb{J}}\frac{1}{h}(\underset{\sim}{W}_{n+1} - \underset{\sim}{W}_n) + [(1-\gamma)\underset{\sim}{W}_n + \gamma\underset{\sim}{W}_{n+1}] \times \underset{\sim}{\mathbb{J}}[(1-\gamma)\underset{\sim}{W}_n + \gamma\underset{\sim}{W}_{n+1}] = \underset{\sim}{0}.$$

$$[\underset{\sim}{\Pi}_{n+1} - \underset{\sim}{\Pi}_n] + h[(1-\gamma)\underset{\sim}{W}_n + \gamma\underset{\sim}{W}_{n+1}] \times [(1-\gamma)\underset{\sim}{\Pi}_n + \gamma\underset{\sim}{\Pi}_{n+1}] = \underset{\sim}{0}.$$

- Angular Momentum. We shall take the dot product of the above equation with $[(1-\gamma)\underset{\sim}{\Pi}_n + \gamma\underset{\sim}{\Pi}_{n+1}]$, yielding

$$[\underset{\sim}{\Pi}_{n+1} - \underset{\sim}{\Pi}_n] \cdot [(1-\gamma)\underset{\sim}{\Pi}_n + \gamma\underset{\sim}{\Pi}_{n+1}] = 0.$$

$$(1-\gamma)\underset{\sim}{\Pi}_{n+1}\cdot\underset{\sim}{\Pi}_n + \gamma\|\underset{\sim}{\Pi}_{n+1}\|^2 - (1-\gamma)\|\underset{\sim}{\Pi}_n\|^2 - \gamma\underset{\sim}{\Pi}_n\cdot\underset{\sim}{\Pi}_{n+1} = 0$$

$$\gamma\|\underset{\sim}{\Pi}_{n+1}\|^2 = (1-\gamma)\|\underset{\sim}{\Pi}_n\|^2 + (2\gamma-1)\underset{\sim}{\Pi}_n\cdot\underset{\sim}{\Pi}_{n+1} .$$

Clearly, $\|\underset{\sim}{\Pi}_{n+1}\|^2 = \|\underset{\sim}{\Pi}_n\|^2$ iff $\gamma = 1/2$. ✓

- Energy. We shall take the dot product of the same equation with $[(1-\gamma)\underset{\sim}{W}_n + \gamma\underset{\sim}{W}_{n+1}]$, yielding

$$[\underset{\sim}{\Pi}_{n+1} - \underset{\sim}{\Pi}_n] \cdot [(1-\gamma)\underset{\sim}{W}_n + \gamma\underset{\sim}{W}_{n+1}] = 0$$

$$(1-\gamma)\underset{\sim}{\Pi}_{n+1}\cdot\underset{\sim}{W}_n + \gamma\underset{\sim}{\Pi}_{n+1}\cdot\underset{\sim}{W}_{n+1} - (1-\gamma)\underset{\sim}{\Pi}_n\cdot\underset{\sim}{W}_n - \gamma\underset{\sim}{\Pi}_n\cdot\underset{\sim}{W}_{n+1} = 0$$

Now, the kinetic energy of the system is $H = \frac{1}{2}\underset{\sim}{W}\cdot\underset{\sim}{\mathbb{J}}\underset{\sim}{W}$.

NEXT →

Thus, we have

$$2\gamma H_{n+1} = 2(1-\gamma) H_n + \gamma\, \mathbf{\Pi}_n \cdot \mathbf{W}_{n+1} - (1-\gamma)\, \mathbf{\Pi}_{n+1} \cdot \mathbf{W}_n .$$

$$2\gamma H_{n+1} = 2(1-\gamma) H_n + \gamma\, \mathbb{J}\mathbf{W}_n \cdot \mathbf{W}_{n+1} + (\gamma-1)\, \mathbb{J}\mathbf{W}_{n+1} \cdot \mathbf{W}_n$$

Now, $\mathbb{J}$ is symmetric so $\mathbb{J}\mathbf{W}_n \cdot \mathbf{W}_{n+1} = \mathbf{W}_n \cdot \mathbb{J}\mathbf{W}_{n+1}$. Thus,

$$2\gamma H_{n+1} = 2(1-\gamma) H_n + (2\gamma - 1)\, \mathbf{W}_n \cdot \mathbf{\Pi}_{n+1} .$$

Clearly, $H_{n+1} = H_n$ iff $\gamma = 1/2$. ✓

$\boxtimes$

This result is in slight contradiction with the paper of SIMO & WONG [1991] where it is stated that the only choice of parameters leading to both conservation of energy and conservation of the norm of angular momentum is $\gamma = 1/2$ and $\beta = 1/4$. However, we have shown that the choice of β has no effect on these conservation properties.

SIMO & WONG [1991] also claim the following:

1. The algorithm is convergent, and second order accurate for $\gamma = 1/2$.
2. The algorithm is unconditionally stable for $\gamma \geq 1/2$ and $\beta \geq 1/4$.

These claims are not proven in the paper, but appear to be based on results for a similar algorithm presented in SIMO & VU-QUOC [1988].

While we have shown that certain conservation properties exist independen- of the choice of β, it may still be the case that the β-paramter is critical to the convergence and accuracy of the algorithm. The choice of β directly affects the $\mathbf{\Theta}$-variable, and thus directly affects the configuration update for $\mathbf{\Lambda}_{n+1}$. It is possible that a choice of $\beta \neq 1/4$ will result in a loss of accuracy and convergence for $\mathbf{\Theta}$ and $\mathbf{\Lambda}$, and thus produce an algorithm which yields quite poor results.

In general, this algorithm does not conserve the total spatial angular momentum relative to the center of mass. While $\|\mathbf{\Pi}_{n+1}\| = \|\mathbf{\Pi}_n\|$ under zero external torque incremental motions, in general $\mathbf{\Pi}_{n+1} \neq \mathbf{\Pi}_n$.

PART 4: A Modified Energy and Momentum Conserving Algorithm.

Recall that we have the balance equation

$$\dot{\underset{\sim}{\pi}} = \overline{\underset{\sim}{\Lambda}\underset{\sim}{\mathbb{J}}\underset{\sim}{W}}^{\,\cdot} = \underset{\sim}{\overline{m}} .$$

We may integrate this expression over $[t_n, t_{n+1}]$ which yields the discrete conservation law

$$\underset{\sim}{\Pi}_{n+1} - \underset{\sim}{\Pi}_n = \underset{\sim}{\Lambda}_{n+1}\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_{n+1} - \underset{\sim}{\Lambda}_n\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n = \int_{t_n}^{t_{n+1}} \overline{m}(t)\, dt .$$

The evaluation of the integral on the right-hand side of the above equation by a generalized type of mid-point rule leads to the algorithm presented below.

Consider the following algorithm ALGO-C1 :

Step 1. Define the configuration update exactly as in ALGO-1 by

$$\underset{\sim}{\Lambda}_{n+1} = \underset{\sim}{\Lambda}_n \exp[\hat{\underset{\sim}{\theta}}] .$$

Step 2. Define the convected angular velocity in terms of the rotation vector $\underset{\sim}{\Theta}$ as

$$\underset{\sim}{W}_{n+1} = \frac{\gamma}{\beta h}\underset{\sim}{\Theta} - \underset{\sim}{W}_n + \left(2 - \frac{\gamma}{\beta}\right)\left(\underset{\sim}{W}_n + \tfrac{1}{2} h \underset{\sim}{A}_n\right)$$

Step 3. Formulate the momentum balance equation in <u>conservation</u> form

$$\underset{\sim}{\Lambda}_{n+1}\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_{n+1} - \underset{\sim}{\Lambda}_n\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n = h\,\overline{m}_{n+\alpha}$$

where a possible choice for $\alpha \in (0,1]$ is

$$\alpha = \begin{cases} \beta/\gamma , & \text{if } \beta/\gamma \le 1 \\ 1 , & \text{otherwise} \end{cases}$$

Step 4. Update the convected angular acceleration as

$$\underset{\sim}{A}_{n+1} = \frac{1}{\gamma h}\left[\underset{\sim}{W}_{n+1} - \underset{\sim}{W}_n\right] + \left(1 - \frac{1}{\gamma}\right)\underset{\sim}{A}_n .$$

SIMO & WONG [1991] state the following:

1. By construction, for zero external applied torque in the interval $[t_n, t_{n+1}]$, the algorithm ALGO-C1 conserves the total spatial angular momentum relative to the center of mass (Π) in the interval $[t_n, t_{n+1}]$. This is clear from momentum balance equation in conservation form

$$\Pi_{n+1} - \Pi_n = \Lambda_{n+1} \mathbb{J} W_{n+1} - \Lambda_n \mathbb{J} W_n = h \bar{m}_{n+\alpha} = 0$$

when $\bar{m}_{n+\alpha} = 0$.

2. For $\beta/\gamma = 1/2$, the algorithm conserves energy when the applied torque in the time interval is zero. We prove this below.
3. For a choice of paramters $\alpha = \beta/\gamma = 1/2$, the configuration and velocity updates, as well as the momentum balance equation, are independent of the convected angular accelerations A_n and A_{n+1}. The algorithm becomes defined entirely in terms of $\{\Theta, W\}$ and we simply have a decoupled update procedure for the convected acceleration. Thus, choosing $\alpha = 1/2$ would appear to reduce the complexity of the numerical implementation of the algorithm.
4. For $\alpha = 1/2$, numerical experiments indicate that the value $\gamma = 1$ (which implies $\beta = 1/2$) yields the best results for the convected acceleration. This choice gives

$$A_{n+1} = \frac{1}{h}\left[W_{n+1} - W_n \right]$$

making the acceleration update insensitive to error propagation via A_n.

5. The algorithm is second order accurate in configuration and velocities for the optimal choice $\alpha = 1/2$. They prove this by comparing ALGO-C to ALGO-1 (with $\beta = 1/4, \gamma = 1/2$) and showing that the two differ by terms of $O(h^3)$. Since ALGO-1 is second order accurate when $\beta = 1/4$ and $\gamma = 1/2$, ALGO-C1 must be second order accurate when $\alpha = 1/2$.

Theorem 3: Let the applied torque in the interval $[t_n, t_{n+1}]$ be zero. Then the total energy is conserved by ALGO-C1 if and only if $\beta/\gamma = 1/2$. (Note: $\beta \neq 0$ and $\gamma \neq 0$).

Proof: First, for simplicity we write the velocity update as

$$W_{n+1} = \frac{\gamma}{\beta h} \Theta - W_n + (2 - \gamma/\beta) W_n^*$$

$$W_n^* = W_n + \tfrac{1}{2} h A_n .$$

Now, we write

$$\begin{aligned} w_{n+1} &= \Lambda_{n+1} W_{n+1} \\ &= \Lambda_n \exp[\hat{\Theta}] \left[\frac{\gamma}{\beta h} \Theta - W_n + (2 - \gamma/\beta) W_n^* \right] \\ &= \Lambda_n \left[\frac{\gamma}{\beta h} \Theta - \exp[\hat{\Theta}] W_n + (2 - \gamma/\beta) \exp[\hat{\Theta}] W_n^* \right]. \end{aligned}$$

NEXT →

$$\underset{\sim}{w}_{n+1} = \Lambda_n\left[\underset{\sim}{W}_{n+1} + \underset{\sim}{W}_n - (2-\gamma/\beta)\underset{\sim}{W}_n^* - \exp[\hat{\theta}]\underset{\sim}{W}_n + (2-\gamma/\beta)\exp[\hat{\theta}]\underset{\sim}{W}_n^*\right]$$

$$= \Lambda_n\left[\underset{\sim}{W}_{n+1} + \underset{\sim}{W}_n - \exp[\hat{\underset{\sim}{\theta}}]\underset{\sim}{W}_n + (\exp[\hat{\underset{\sim}{\theta}}]-1)(2-\gamma/\beta)W_n^*\right]$$

$$= \Lambda_n\underset{\sim}{W}_{n+1} + \Lambda_n\underset{\sim}{W}_n - \Lambda_{n+1}\underset{\sim}{W}_n + (\Lambda_{n+1}-\Lambda_n)(2-\gamma/\beta)\underset{\sim}{W}_n^*.$$

$$= \Lambda_n\underset{\sim}{W}_{n+1} + \underset{\sim}{w}_n - \Lambda_{n+1}\underset{\sim}{W}_n + (\Lambda_{n+1}-\Lambda_n)(2-\gamma/\beta)\underset{\sim}{W}_n^*.$$

Next, from the above we write

$$\underset{\sim}{w}_{n+1} - \underset{\sim}{w}_n = \Lambda_n\underset{\sim}{W}_{n+1} - \Lambda_{n+1}\underset{\sim}{W}_n + [\Lambda_{n+1}-\Lambda_n](2-\gamma/\beta)\underset{\sim}{W}_n^*.$$

Now, we have the energy and momentum relationships

$$2(H_{n+1} - H_n) = \underset{\sim}{\Pi}_{n+1}\cdot\underset{\sim}{w}_{n+1} - \underset{\sim}{\Pi}_n\cdot\underset{\sim}{w}_n$$
$$\underset{\sim}{\Pi}_{n+1} = \underset{\sim}{\Pi}_n \text{ (by construction)}$$

We next can write, noting that $\underset{\sim}{\Pi}_{n+1} = \underset{\sim}{\Pi}_n$,

$$2(H_{n+1} - H_n) = \Lambda_n\underset{\sim}{W}_{n+1}\cdot\underset{\sim}{\Pi}_n - \Lambda_{n+1}\underset{\sim}{W}_n\cdot\underset{\sim}{\Pi}_{n+1} + (2-\gamma/\beta)\underset{\sim}{\Pi}_{n+1}\cdot[\Lambda_{n+1}-\Lambda_n]\underset{\sim}{W}_n^*$$

$$= \underset{\sim}{W}_{n+1}\cdot\underset{\sim}{\Pi}_n - \underset{\sim}{W}_n\cdot\underset{\sim}{\Pi}_{n+1} + (2-\gamma/\beta)[\underset{\sim}{\Pi}_{n+1} - \underset{\sim}{\Pi}_n]\cdot\underset{\sim}{W}_n^*$$

$$= \cancel{\underset{\sim}{W}_{n+1}\cdot\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n} - \cancel{\underset{\sim}{W}_n\cdot\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_{n+1}} + (2-\gamma/\beta)[\underset{\sim}{\Pi}_{n+1} - \underset{\sim}{\Pi}_n]\cdot\underset{\sim}{W}_n^*$$

$$= (2-\gamma/\beta)(\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_{n+1} - \underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n)\cdot\underset{\sim}{W}_n^*.$$

Clearly, $H_{n+1} = H_n$ iff $\gamma/\beta = 2$.

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We now include, for completeness, the simplifications gained in ALGO-C1 if we choose $\alpha = \beta/\gamma = 1/2$. Recall that, for ALGO-C1,

$$\Lambda_{n+1} = \Lambda_n\exp[\hat{\underset{\sim}{\theta}}]$$

$$\underset{\sim}{W}_{n+1} = \frac{\gamma}{\beta h}\theta - \underset{\sim}{W}_n + (2-\gamma/\beta)\underset{\sim}{W}_n^*$$

$$\Lambda_{n+1}\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_{n+1} - \Lambda_n\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n = h\overline{m}_{n+\alpha}.$$

We may substitute the update equations in the momentum balance equation.

$$\Lambda_n\exp[\hat{\underset{\sim}{\theta}}]\underset{\sim}{\mathbb{J}}\left[\frac{\gamma}{\beta h}\underset{\sim}{\theta} - \underset{\sim}{W}_n + (2-\gamma/\beta)W_n^*\right] - \Lambda_n\underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n = h\underset{\sim}{\overline{m}}_{n+\alpha}.$$

$$\exp[\hat{\underset{\sim}{\theta}}]\underset{\sim}{\mathbb{J}}\left[\frac{\gamma}{\beta h}\underset{\sim}{\theta} - \underset{\sim}{W}_n + (2-\gamma/\beta)W_n^*\right] - \underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n = \Lambda_n^T h\underset{\sim}{\overline{m}}_{n+\alpha}$$

This is clearly a non-linear equation in $\underset{\sim}{\theta}$. If we choose $\alpha = \beta/\gamma = 1/2$, it simplifies to

$$\exp[\hat{\underset{\sim}{\theta}}]\underset{\sim}{\mathbb{J}}\left[\frac{1}{2h}\underset{\sim}{\theta} - \underset{\sim}{W}_n\right] - \underset{\sim}{\mathbb{J}}\underset{\sim}{W}_n - \Lambda_n^T h\underset{\sim}{\overline{m}}_{n+1/2} = 0.$$

The algorithm ALGO-C1 would appear to be superior to the algorithm ALGO-1. It posesses all the properties of ALGO-1, but in addition conserves the angular momentum vector as well as the norm of the angular momentum.

We see that the fundamental difference between the two algorithms is that ALGO-1 uses the rate of momentum balance equation

$$\underset{\sim}{\mathbb{J}}\underset{\sim}{A} + \underset{\sim}{W} \times \underset{\sim}{\mathbb{J}}\underset{\sim}{W} = \underset{\sim}{\Lambda}^T \underset{\sim}{\bar{m}}$$

while ALGO-C1 uses the momentum balance equation in conservation form

$$\underset{\sim}{\Lambda}_{n+1} \underset{\sim}{\mathbb{J}} \underset{\sim}{W}_{n+1} - \underset{\sim}{\Lambda}_n \underset{\sim}{\mathbb{J}} \underset{\sim}{W}_n = \int_{t_n}^{t_{n+1}} \underset{\sim}{\bar{m}}\, dt .$$

The fact that ALGO-C1 uses the conservation equation rather than the rate equation is what enables the algorithm to conserve the spatial angular momentum during torque-free incremental motions.

Finally, with respect to the numerical implementation of the algorithm, the quaternian parameterization of SO(3) appears to be the simplest and most efficient method for manipulating rotation vectors and elements of SO(3). This fact is elaborated upon in appendices I and II of SIMO & WONG [1991]. See also SIMO & VU-QUOC [1988].

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