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Geometric Pseudospectral Method on Lie Group with application to 3D Pendulum

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***Abstract*—General pseudospectral method is extended to Lie group by virtue of equivariant map for solving rigid dynamics on Lie group. In particular, for the problem of structural characteristics of the dynamics system can not be conserved by using general pseudospectral method directly on Lie group, the differential equation evolving on the Lie group is transformed to an equivalent differential equation evolving on a Lie algebra on which general pseudospectral method is used, so that the numerical flow of rigid body dynamics is ensured to stay on Lie group. Furthermore, structural conservativeness and numerical stabilities of this method are validated and analyzed by simulation on a 3D pendulum in comparison with using pseudospectral method directly on Lie group.**

Keywords–geometric pseudospectral method; Lie group; Equivariant map; 3D pendulum

I. INTRODUCTION

The dynamics of a rigid body has intrinsic invariant properties, for example, energy, momentum, symplecticity, structure of configuration, etc. The invariants often manifest through geometric characteristics of exact flow, such as area preservation, volume preservation. Preservation of geometric characteristics of the corresponding numerical flow not only produce an improved qualitative behavior, but also allows for a more accurate long-time integration than with general-purpose methods [1]. Therefore, developing numerical method with preservation of geometric characteristics for solving differential equation of rigid body dynamics is very important.

Finite difference methods (1950s), finite element methods (1960s) and spectral methods (1970s) are three major technologies for numerical solution of differential equations. Spectral methods are widely used in fluid mechanics, quantum mechanics, linear and nonlinear waves, aerospace, and other fields by virtue of its high accuracy, spectral(or exponential) convergence rates, and requirement for less computer memory under the same precision condition, etc[2]. According to the different choice of test functions or error, spectral method is divided into Galerkin, tau and collocation[3]. Among them, collocation method, also known as pseudospectral method, is advantageous because the coefficients of the Lagrange polynomials are equal to the value of the approximating polynomial at the collocation points[3]. However, when applied to rigid body dynamics directly, it can not conserve geometric properties. Thereby, how to conserve its geometric properties, and extend it to dynamics system on Lie group is the main topic in this paper.

To our knowledge, R. Moulla et al[4] was the first to propose the concept of ‘geometric pseudospectral method’. They suggested a polynomial pseudospectral method that preserves the geometric structure of port-Hamiltonian systems, the phenomenological laws and the conservation laws without introducing any uncontrolled numerical dissipation. However, their method was designed only for port-Hamiltonian systems having a special structure, that is, the Dirac structure. Therefore, it can not be directly extended to the general system. [5] compared pseudospectral method and discrete geometric method for modeling quantization effects in nanoscale electron devices; they confirmed that pseudospectral methods can achieve the spectral accuracy but are mainly suitable for simple geometries.

In this paper, drawing on Kenth Engø’s equivariant map[6], we extend pseudospectral method to Lie group, and make the method have symplecticity by proper choice of collocation points. Second, we analyze Lie group structural conservativeness, energy conservation, and momentum conservation of this method by simulation on a 3D pendulum in comparison with using general pseudospectral method on Lie group directly.

This paper is organized as follows. For completeness, the basic idea of the pseudospectral method is roughly given in Section II. Geometric pseudospectral method on Lie group is developed in Section III, in subsection III.A, we briefly describe differential equation on Lie group, in subsection III.B, we apply general pseudospectral method to differential equation on Lie group by the equivariant map, and symplectic collocation points are selected in next subsection. In Section IV, we validate and analyze structural conservativeness and numerical stabilities of this method by simulation on a 3D pendulum in comparison with general pseudospectral method.

II. PSEUDOSPECTRAL METHOD

Consider differential equation on Euclidean space $\mathbb{R}^n$

$$\dot{y}(t) = f\left(t, y(t)\right), \quad y(t_0) = y_0 \in \mathbb{R}^n \tag{1}$$

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First, we equally divide a time interval $\left[t_0, t_f\right]$ into several subintervals $\left[t_i, t_{i+1}\right]$. Let $\tau_0 < \tau_1 < \cdots < \tau_N$ be collocation points, where $\tau_0 = t_i$ and $\tau_N = t_{i+1}$, subjected to

$$\tau_j = t_i + h_i \alpha_j, \quad 0 < \alpha_j < 1, \quad j = 1, \ldots, N \tag{2}$$

Next, we select the following N th degree Lagrange interpolation polynomial for approximating the solution $\mathrm{y}(t)$ of (3),

$$\mathrm{y}(t) \approx \mathrm{Y}(t) = \sum_{i=0}^{N} \mathrm{c}_i L_i(t) \tag{3}$$

where the function $L_i(t) = \prod_{j=0, j\neq i}^{N} \frac{t-\tau_j}{\tau_i - \tau_j}, i = 1, \ldots, N$ is Lagrange polynomials, satisfying the isolation property,

$$L_i(\tau_j) = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \tag{4}$$

Equation (3) together with the isolation property leads to the fact that,

$$\mathrm{c}_i = \mathrm{y}(\tau_i) \tag{5}$$

thus, $\mathrm{Y}(\tau_i) = \mathrm{y}(\tau_i)$.

Finally, we describe the discretized dynamics as defect constraints[7],

$$\varsigma_j = \dot{\mathrm{Y}}(\tau_j) - f\left(\tau_j, y(\tau_j)\right) \tag{6}$$

and use iterative algorithms to approximate $\mathrm{Y}(t)$ in order to obtain the solution of (1) at time t_{i+1},

$$y(t_{i+1}) \approx \mathrm{Y}(t_i + h_i) \tag{7}$$

and refer it as the initial value of $y(t)$ in $\left[t_{i+1}, t_{i+2}\right]$.

According to whether the endpoint as a collocation point, collocation methods fall into three general categories[8]: Gauss methods, neither of the endpoints t_i or t_{i+1} are collocation points; Radau methods, at most one of the endpoints t_i or t_{i+1} is a collocation point; Lobatto methods, both of the endpoints t_i and t_{i+1} are collocation points. Furthermore, according to different selection methods of collocation points, collocation methods can be divided into standard collocation method and orthogonal collocation method. Common collocation points in orthogonal collocation are those obtained from the roots of either Chebyshev polynomials $T_N(t)$ or Legendre polynomials $P_N(t)$ belongs to the orthogonal polynomial[9]. The benefit of using orthogonal collocation over standard collocation is that the quadrature approximation to a definite integral is extremely accurate[7].

III. GEOMETRIC PSEUDOSPECTRAL METHOD ON LIE GROUP

A. *Differential equation on Lie Group*

Differential Equation is presented in the following canonical form

$$\dot{y}(t) = \xi_{\mathcal{M}}\left(t, y(t)\right), \quad y(t_0) = y_0 \in \mathcal{M} \tag{8}$$

$\mathcal{M}$ is a class of homogeneous manifolds, $\xi_{\mathcal{M}}$ is the infinitesimal generator of the left action $\Phi : G \times \mathcal{M} \to \mathcal{M}$ on the Lie group G corresponding to its Lie algebra $\xi \in \mathfrak{g}$,

$$\xi_{\mathcal{M}}(q) = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \Phi_{\exp(t\xi)}(q), \quad \forall q \in \mathcal{M} \tag{9}$$

where $\xi_{\mathcal{M}}$ is a vector field over $\mathcal{M}$, $\Phi_{\exp(t\xi)} : \mathcal{M} \to \mathcal{M}$ is the flow of $\xi_{\mathcal{M}}$, $\exp(t\xi) \in G$ is called the exponential map, it parameterizes G by Lie algebra ξ. What the infinitesimal generator describes is the direction of the motion on the manifold. This is the tangent of the flow and the direction of where to proceed. The solution of a differential equation is an integral curve of the vector field.

An important special case is when G is a subset of $\mathrm{GL}(\mathbb{C}, n)$ the general linear group of all nonsingular $n \times n$ matrics, it is then called a matrix lie group. In the case of matrix Lie group, the exponential operator is just

$$\exp(t\xi) = \sum_{k=0}^{\infty} \frac{1}{k!}(t\xi)^k \tag{10}$$

In remainder of this paper, our study is limited to G is a matrix Lie group, therefore (8) becomes a matrix differential equation. This restriction is for three reasons: first, we will establish the model of the rigid body dynamics evolving on matrix Lie group, followed by Lie group to facilitate the calculation, furthermore, our theory is equally applicable to the general Lie group.

B. *Pseudospectral method on Lie Group*

It is well-known that the solution of (8) stays on $\mathcal{M}$ for all $t \geq t_0$. How to use pseudospectral method for solving differential equation (8) on Lie group, while maintain the important structural feature of the differential equation under discretization of y is the main problem to be solved in this paper.

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As mentioned, infinitesimal generator of group action actually is a vector filed, it governs the equation varies. In Euclidean space $\mathbb{R}^n$, the solution space and the tangent space are linear vector space, classical numerical methods just rely on domain space consisting of vectors, it will conserve the structural characteristics of the differential equations. However, Lie group is a nonlinear manifold, using classical numerical methods directly for solving differential equation on Lie group will not be able to conserve its structural characteristics. [6] indicated that any differential equation in the form of an infinitesimal generator on a homogeneous space is shown to be locally equivalent to a differential equation on the Lie algebra corresponding to the Lie group acting on the homogenous space. Also, Lie algebra of a Lie group is a vector space with the additional structure of a commutator. For the above reasons, the Lie algebra of the Lie group acting on the homogeneous space is the natural choice of space for our pseudospectral method. We will apply the equivariant map to transform the differential equation evolving on the homogeneous space to an equivalent differential equation evolving on a Lie algebra. Next, we will briefly describe the basic idea of equivariant map.

Definition 1(Equivariant map) . Let $\mathcal{M}$ and $\mathcal{N}$ be manifolds and let G be a Lie group which acts on $\mathcal{M}$ by $\Phi_g : \mathcal{M} \to \mathcal{M}$ and on $\mathcal{N}$ by $\Psi_g : \mathcal{N} \to \mathcal{N}$. A smooth map $f : \mathcal{M} \to \mathcal{N}$ is called equivariant with respect to these actions if, for all $g \in G$,

$$f \circ \Phi_g = \Psi_g \circ f \tag{11}$$

that is, the following diagram commutes,

$$\begin{tikzcd} \mathcal{M} \arrow[r, "f"] & \mathcal{N} \\ \mathcal{M} \arrow[u, "\Phi_g"] \arrow[r, "f"'] \arrow[ur, phantom, "(11)"] & \mathcal{N} \arrow[u, "\Psi_g"'] \end{tikzcd}$$

Figure 1. Diagram commutes of equivariant map f

First, from the definition of an action of G on $\mathcal{M}$, we can get an equivariant map $\Phi_y : G \to \mathcal{M}$ with respect to the left translation action L_g of G on itself and an action $\Phi_g, g \in G$ of G on $\mathcal{M}$,

$$\Phi_y \circ L_g = \Phi_g \circ \Phi_y \tag{12}$$

It is known that there is a local coordinate map $f : \mathfrak{g} \to G$ on G, the most typical is exponential map $\exp$. At this point, we need to find an action B_g of G on $\mathfrak{g}$ such that f will be an equivariant map with B_g and the left action of G on itself,

$$f \circ \mathrm{B}_g = L_g \circ f \tag{13}$$

In the case where f is the exponential map, B_g is nothing else than the well-known Baker-Campbell-Hausdorff (BCH) formula,

$$\mathrm{B}_g(u) = \log\left(g \cdot \exp(u)\right) \tag{14}$$

where $\log$ is called the logarithm map. Since composition of two equivariant maps is an equivariant map, we can construct an equivariant map $\Phi_y \circ f$ from $\mathfrak{g}$ to $\mathcal{M}$ with respect to the action B_g on $\mathfrak{g}$ and Φ on $\mathcal{M}$,

$$\begin{tikzcd} \mathfrak{g} \arrow[r, "f"] & G \arrow[r, "\Phi_y"] & \mathcal{M} \\ \mathfrak{g} \arrow[u, "\mathrm{B}_g"] \arrow[r, "f"'] \arrow[ur, phantom, "(13)"] & G \arrow[u, "L_g"'] \arrow[r, "\Phi_y"'] \arrow[ur, phantom, "(12)"] & \mathcal{M} \arrow[u, "\Phi_g"'] \end{tikzcd}$$

Figure 2. Diagram commutes of composition $\Phi_y \circ f$

The theorem 3.6 of [6] stated that if ϕ is an equivariant map, then the infinitesimal generators of the action with respect to the same element $\xi \in \mathfrak{g}$ are ϕ–related vector fields. Thus, the infinitesimal generators of the flows B_g and Φ_g on $\mathfrak{g}$ and $\mathcal{M}$ are $\Phi_y \circ f$–related, that is,

$$\xi_{\mathcal{M}} \circ \Phi_y \circ f = \mathrm{T}\Phi_y \circ \mathrm{T}f \circ \xi_{\mathfrak{g}} \tag{15}$$

Finally, we need to determine what $\xi_{\mathfrak{g}}$ is, and the following theorem gives the conditions that it need to meet.

Theorem 2[6]**.** Let $f : \mathfrak{g} \to G$ be a coordinate map on G and $\Phi_y \circ f$ equivariant with respect to the flows B_g and Φ_g . The infinitesimal generator of B_g satisfying (15), is $\xi_{\mathfrak{g}}(u) = \mathrm{d}f_u^{-1}(\xi)$. $\mathrm{d}f : \mathfrak{g} \to \mathfrak{g}$ is the trivialization $\mathrm{T}f$ defined as $\mathrm{d}f_u = \mathrm{T}R_{f(u)^{-1}} \circ \mathrm{T}f_u$.

The following commutative diagram sums up above processes.

$$\begin{tikzcd} \mathfrak{g} \arrow[r, "\Phi_y \circ f"] & \mathcal{M} & & \mathrm{T}\mathfrak{g} \arrow[r, "\mathrm{T}\Phi_y \circ \mathrm{T}f"] & \mathrm{T}\mathcal{M} \\ \mathfrak{g} \arrow[u, "\mathrm{B}_g"] \arrow[r, "\Phi_y \circ f"'] & \mathcal{M} \arrow[u, "\Phi_g"'] & \Rightarrow & \mathfrak{g} \arrow[u, "\mathrm{d}f_u^{-1}(\xi)"] \arrow[r, "\Phi_y \circ f"'] \arrow[ur, phantom, "(15)"] & \mathcal{M} \arrow[u, "\xi_{\mathcal{M}}(y)"'] \end{tikzcd}$$

Figure 3. Composition $\Phi_y \circ f$ and its infinitesimal generator

According to the different choices of local coordinate map f, function $\mathrm{d}f_u^{-1}(\xi)$ have different forms. In the case where f is the exponential map, the vector field $\mathrm{d}f_u^{-1}$

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on $\mathfrak{g}$ can be represented by following an infinite sum of elements in $\mathfrak{g}$,

$$\mathrm{d}\exp_u^{-1}(\upsilon) = \upsilon - \frac{1}{2}[u,\upsilon] + \sum_{k=2}^{\infty} \frac{B_k}{k!}\left[u,\left[u,\left[\ldots,[u,\upsilon],\ldots\right]\right]\right] \quad (16)$$

where $[\cdot,\cdot]$ is the matrix commutator defined by $[A,B] = AB - BA$, when A and B are matrics, and B_k is the k^{th} Bernoulli number.

$$\frac{B_k}{k!} = \begin{cases} 0, & k \in 2N-1, N \in \mathbb{Z}^+ \\ \frac{1}{12}, \frac{-1}{720}, \frac{1}{30240}, \frac{-1}{1209600}, \ldots & k = 2,4,6,8,\ldots \end{cases}$$

In the case of solution of (8) satisfying the form,

$$y(t) = \exp(u(t))\, y_0 \quad (17)$$

Using the dexp^{-1}, we differentiate (17) and substitute it into (8) to obtain a differential equation for $u(t)$

$$\begin{aligned} \dot{u}(t) &= \mathrm{dexp}_u^{-1}(\xi(t)) \\ &= \xi(t) - \frac{1}{2}\left[u(t),\xi(t)\right] + \frac{1}{12}\left[u(t),\left[u(t),\xi(t)\right]\right] - \ldots \end{aligned} \quad (18)$$

where $u(t_0) = u_0 \in \mathfrak{g}$.

In the general case we can apply Picard iteration to (18), deduce the famous Magnus expansion[10].

$$\begin{aligned} u(t) &= \int_0^t \xi(\tau_1)\,\mathrm{d}\tau_1 \\ &\quad - \frac{1}{2}\int_0^t \left[\xi(\tau_1), \int_0^{\tau_1} \xi(\tau_2)\,\mathrm{d}\tau_2\right]\mathrm{d}\tau_1 + \ldots \end{aligned} \quad (19)$$

Now, we can use general pseudospectral method on $u(t)$ without any concerns. We approximate function ξ in vector space $\mathfrak{g}$ by virtue of Lagrange polynomials at $c_1, c_2, \ldots, c_v$,

$$\xi(t, y(t)) \approx \sum_{i=1}^{s} L_i\left(\frac{t-t_n}{h}\right)\xi_i \quad (18)$$

where

$$L_i(t) = \prod_{\substack{k=1 \\ k\neq i}}^{s} \frac{t - c_k}{c_i - c_k} \quad (19)$$

$$\xi_i \approx \xi\left(t_n + c_i h, y(t_n + c_i h)\right), \quad i = 1,\ldots,s \quad (20)$$

Finally, we substitute (18) into (19) to obtain $u(t)$ and evaluate (17) to obtain $y(t)$. Then, solving (8) on homogeneous manifold $\mathcal{M}$ is equivalent to solving differential equation on a Lie algebra $\mathfrak{g}$.

C. Choice of symplectic collocation points

As mentioned, there are a variety of options on the choice of collocation points, for example, Gauss-Legendre points, Chebyshev-Gauss-Lobatto points, etc. In order to make pseudospectral method have symplecticity, we need to consider the relationship between the choice of collocation points and symplecticity. [1] stated that the Gauss collocation methods are symplectic. Therefore, we select Gauss-Legendre points as our collocation points in this paper.

IV. Numerical Simulation

$\mathrm{SO}(3) = \left\{R_{ab} \in \mathbb{R}^{3\times3} \middle| R_{ab}R_{ab}^T = I, \det R_{ab} = +1\right\}$ is called the special orthogonal group, a special class of matrix Lie group, whose elements meet to special nature $R_{ab}R_{ab}^T = I$. Therefore, it is often to validate the structural features of algorithms on $\mathrm{SO}(3)$. The configuration of 3D pendulum just is $\mathrm{SO}(3)$, next, it will be used as a simulation object for this method in comparison with the other methods[11].

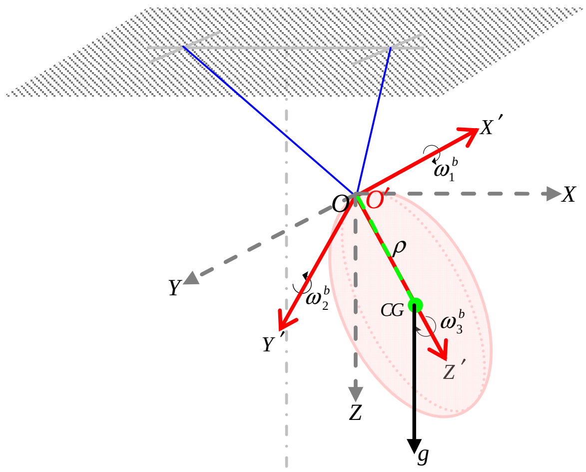

Figure 4. A schematic of 3D rigid pendulum

A. Mathematical models for a 3D rigid pendulum

$$\dot{R}_{ab} = R_{ab}\hat{\omega}_{ab}^b \quad (21)$$

$$\dot{\omega}_{ab}^b = J^{-1}\left(-\omega_{ab}^b \times J\omega_{ab}^b\right) + mgJ^{-1}\left(\rho \times R_{ab}^T e_3^a\right) \quad (22)$$

where $R_{ab} := q$ is a generalized coordinate of rotation angular configuration of the body-fixed coordinate frame $\{b\}$ relative to the inertial coordinate frame $\{a\}$, m is the mass of pendulum, J is the moment of inertia of pendulum, ω_{ab}^b

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is the angular velocity in the body-fixed coordinate frame, ρ is body-fixed vector from the pivot to the center of mass of the pendulum, $e_3^a = [0 \quad 0 \quad 1]^T$ denotes the direction vector of gravity in inertial coordinate frame.

B. Geometric pseudospectral method

We take implicit pseudospectral method based on Gauss-Legendre collocation points, and the step is taken as $h = 0.05$, let c_1 and c_2 be the Gauss-Legendre points,

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \ c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6} \tag{23}$$

and evaluate ξ at these collocation points in $[t_n, t_n + h]$,

$$\xi_1 = \xi(t_n + c_1 h), \ \xi_2 = \xi(t_n + c_2 h) \tag{24}$$

A 4[th] order approximation to $u(t)$ is then given as,

$$u^{[4]}(t) = \frac{1}{2} h(\xi_1 + \xi_2) - \frac{\sqrt{3}}{12} h^2 [\xi_1, \xi_2] \tag{25}$$

The solution y_{n+1} is updated according to

$$y_{n+1} = \Phi\left(\exp\left(u^{[4]}(t)\right), y_n\right) \tag{26}$$

where exp is matrix exponential operator (10).

Notes that the tangent space of a Lie algebra ξ is isomorphism to Euclidean space $\mathbb{R}^n$. Thus, we can directly apply general pseudospectral method to (22) for solving ξ_1 and ξ_2. Specific algorithm process is shown in Fig. 5.

Algorithm 1
Step 1. Initialization:
Initialize attitude R_0, angular velocity ω_0;
Step 2. Main loop
Step 2.1. Evaluate Lie algebra $\xi_1 := \omega_{ab}^b(t_n + c_1 h)$
Evaluate Gauss differential matrix D_1 in $[t_n, t_n + c_1 h]$,
Use Seidal type iteration for solving following dynamics equation, obtain the Lie algebra ξ_1,
$\dot{\xi}_1 = J^{-1}\left(-\omega_{ab}^b \times J\omega_{ab}^b\right) + mgJ^{-1}\left(\rho \times R_{ab}^T e_3^a\right)$
Step 2.2. Evaluate Lie algebra $\xi_2 := \omega_{ab}^b(t_n + c_2 h)$
Evaluate Gauss differential matrix D_2 in $[t_n, t_n + c_2 h]$,
Use Seidal type iteration for solving following dynamics equation, obtain the Lie algebra ξ_2,
$\dot{\xi}_2 = J^{-1}\left(-\omega_{ab}^b \times J\omega_{ab}^b\right) + mgJ^{-1}\left(\rho \times R_{ab}^T e_3^a\right)$
Step 2.3. Evaluate 4[th] order approximation of $u(t)$
$u^{[4]}(t) = \frac{1}{2} h(\xi_1 + \xi_2) - \frac{\sqrt{3}}{12} h^2 [\xi_1, \xi_2]$
Step 2.3. Update attitude R_{n+1} and angular velocity ω_{n+1}
$R_{n+1} = R_n \exp\left(u^{[4]}(t)\right)$, $\omega_{n+1} = R_{n+1}\omega_n$
Step 3. End Loop.

Figure 5. 4[th] order implicit geometric pseudospectral algorithm

C. Results and analysis

The properties of a 3D pendulum are presented at Table I.

TABLE I. THE PROPERTIES OF 3D RIGID PENDULUM[12]

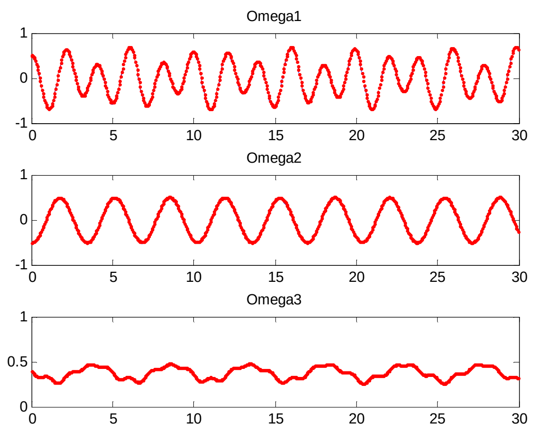
Time	$t = [0, 30]$ s
Mass	$m = 1$ kg
Body-fixed vector	$\rho = [0, 0, 1]$ m
Moment of inertia	$J = \mathrm{diag}[1, 2.8, 2]$ kg • m²
Initial attitude	$R_{ab}(0) = I_{3\times3}$
Initial angular velocity	$\omega_{ab}^b(0) = [0.5, -0.5, 0.4]^T$ rad/s

Simulation results are presented in Fig. 6, where the top figure shows time histories of the angular velocity, and the bottom figure shows the variation of the $SO(3)$ error (27), the total energy (28) and the angular momentum around the vertical axis (29).

$$\text{error} = \left\| I_{3\times3} - R^T R \right\|_\infty \tag{27}$$

$$\text{energy} = \frac{1}{2}\left(J\omega_{ab}^b\right)^T J\left(J\omega_{ab}^b\right) - mge_3^T R\rho \tag{28}$$

$$\text{momentum} = e_3^T RJ\omega_{ab}^b \tag{29}$$



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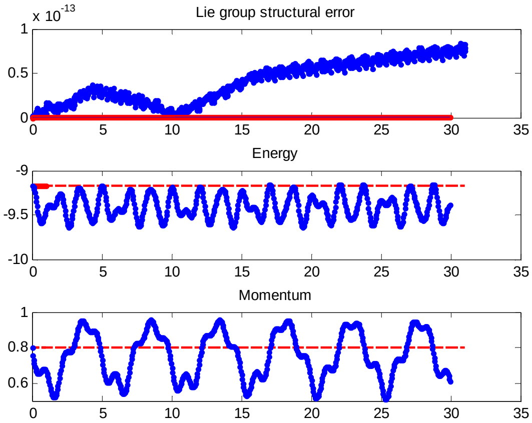

Figure 6. Simulation results of 3D pendulum: (a) angular velocity, (b) the $SO(3)$ error, total energy, and momentum. (general pseudospectral: blue, geometric pseudospectral: red)

The result show that general pseudospectral method can not conserve energy and momentum, while the $SO(3)$ error are about 10^{-13} and increase as the simulation time increases. For geometric pseudospectral method, the $SO(3)$ error are up to machine precision 10^{-16}, and the method presents a good long-time behavior.

V. CONCLUSION

Aiming at can not conserve structural properties of dynamics system by applying general pseudospectral method onto Lie group directly, we transform the differential equation evolving on the Lie group to an equivalent differential equation evolving on a Lie algebra, and use general pseudospectral method on the equivalent differential equation, so that ensure that numerical flow of rigid body dynamics stay on Lie group. We will validate our method on more general homogeneous manifolds, such as, special Euclidean group, spheres, tori, Stiefel and Grassmann manifolds, etc.

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