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ORIGINAL ARTICLE

Lie group variational integrators for the full body problem in orbital mechanics

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Abstract Equations of motion, referred to as full body models, are developed to describe the dynamics of rigid bodies acting under their mutual gravitational potential. Continuous equations of motion and discrete equations of motion are derived using Hamilton's principle. These equations are expressed in an inertial frame and in relative coordinates. The discrete equations of motion, referred to as a Lie group variational integrator, provide a geometrically exact and numerically efficient computational method for simulating full body dynamics in orbital mechanics; they are symplectic and momentum preserving, and they exhibit good energy behavior for exponentially long time periods. They are also efficient in only requiring a single evaluation of the gravity forces and moments per time step. The Lie group variational integrator also preserves the group structure without the use of local charts, reprojection, or constraints. Computational results are given for the dynamics of two rigid dumbbell bodies acting under their mutual gravity; these computational results demonstrate the superiority of the Lie group variational integrator compared with integrators that are not symplectic or do not preserve the Lie group structure.

Keywords Symplectic integrator · Variational integrator · Lie group method · Full rigid body problem

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1 Introduction

The full body problem in orbital mechanics treats the dynamics of non-spherical rigid bodies in space interacting under their mutual potential. Since the mutual gravitational potential of distributed rigid bodies depends on both the position and the attitude of the bodies, the translational and the rotational dynamics are coupled in the full body problem. For example, the orbital motion and the attitude dynamics of a very large spacecraft in the Earth's gravity field are coupled, and the dynamics of a binary asteroid pair, with non-spherical mass distributions of the bodies, involves coupled orbital and attitude dynamics. Recently, interest in the full body problem has increased, as it is estimated that up to 16% of near-earth asteroids are binaries (Margot et al. 2002).

These full body dynamics arise from Lagrangian and Hamiltonian mechanics; they are characterized by symplectic, momentum and energy preserving properties. These geometric features determine the qualitative behavior of the full body dynamics, for example stability conditions (Scheeres 2002), and they can serve as a basis for further theoretical study of the full body problem. The configuration space of the full body dynamics has a Lie group structure referred to as the special Euclidean group, SE(3). The representation used for the attitude of the bodies should be globally defined since the complicated dynamics would require frequent changes of coordinates when using representations that are only locally defined.

However, general numerical integration methods, including the widely used explicit (non-symplectic) Runge-Kutta schemes, neither preserve the Lie group structure nor these geometric properties. (Hairer et al 2006). They fail to preserve the conserved quantities such as total energy and angular momentum, which determine the qualitative behavior of the full body dynamics. Attitude errors tend to accumulate, and this attitude degradation causes significant errors in the computation of gravitational forces and moments. The accuracy of such general purpose integrators also rapidly degrades as the simulation time increases (Fahnestock et al 2006).

Moser and Veselov (1991), Wendlandt and Marsden (1997) developed numerical integrators for a free rigid body by imposing an orthogonal constraint on the attitude variables, and by using unit quaternions, respectively. The idea of using the Lie group structure and the exponential map to numerically compute rigid body dynamics arises in the work of Simo et al. (1992), and in the work by Krysl (2005). Marsden et al. (1999) and Marsden et al. (2000) introduce discrete Euler–Poincaré and Lie–Poisson equations, where the discrete dynamics on a Lie group are reduced to the dynamics on the corresponding Lie algebra in the absence of potential. Lie-Poisson integrators have been developed by splitting the Hamiltonian into separate integrable terms for an elliptical body (Touma and Wisdom, 1994; Breiter et al. 2005a) and for the secular spin dynamics of a rigid body (Breiter et al. 2005b).

Variational integrators and Lie group methods provide a systematic method of constructing structure-preserving numerical integrators. The idea of the variational approach is to discretize Hamilton's principle (Marsden and West 2001). The numerical integrator obtained from discrete Hamilton's principle exhibits excellent energy properties (Hairer 1994), conserves first integrals associated with symmetries by a discrete version of Noether's theorem, and preserves the symplectic structure. Lie group methods consist of numerical integrators that preserve the geometry of the configuration space by automatically remaining on the Lie group (Iserles et al. 2000).

In this paper, the Lie group approach is explicitly adopted in the context of a variational integrator for the full rigid bodies problem. This is an extension of the geometric integrator for rigid body attitude dynamics on the rotation group SO(3) by Lee et al. (2005) to attitude and translational dynamics on the special Euclidean group SE(3), and here reduced equations of motion are also developed in relative coordinates. This unified integrator, hereafter referred to as the Lie Group Variational Integrator (or LGVI for short), is symplectic and momentum preserving, and it exhibits good total energy behavior for exponentially long time periods. It also preserves the Euclidian Lie group structure without the use of local charts, reprojection, or constraints. The exact geometric properties of the discrete flow not only provides improved qualitative behavior, but also results in accurate long-time simulation. This provides a uniform method that can be applied to rigid bodies acting under any type of potential that depends on the position and the attitude, but we focus on the application to astrodynamics problems with the gravitational potential in this paper. This development has been presented in Lee et al. (2007); the present paper emphasizes the development of this approach for full body problems in orbital mechanics and the special computational features of this approach for full body problems in orbital mechanics. In addition, we make a computational comparison between the Lie group variational integrator to other geometric integrators such as symplectic Runge-Kutta method and Lie group method (Hairer et al. 2006).

Numerical simulation of the full body problem involves a large computational burden in computing mutual gravitational forces and moments, which are usually represented by a finite series approximation for the double volume integration (Werner and Scheeres 2005). The forces and moments must be reevaluated for any position change or any orientation change, not only at each time step but at each sub-step involved in the differencing scheme behind any general purpose numerical integrator. Therefore the choice of numerical integrator can significantly amplify the burden of computing the gravity forces and moments. The LGVI minimizes the computational burden in the sense that it requires only one force and torque evaluation per integration step for second order accuracy. It has been shown that the LGVI yields a numerically efficient computational algorithm for the full body problem (Fahnestock et al. 2006).

This paper is organized as follows. The continuous equations of motion and Lie group variational integrators are derived in Sects. 2 and 3, respectively. Numerical simulations for two rigid dumbbell bodies are presented in Sect. 4.

2 Continuous time full body models

Maciejewski (1995) presented the continuous equations of motion for the full body problem in Hamiltonian form without providing a formal derivation. Here, we show that the equations can be derived from Hamilton's variational principle using the Lagrangian formalism. The proper form for the variations of Lie group elements in the configuration space leads to a systematic derivation of the equations of motion. In this section, we summarize those procedures; the Lie group variational integrators presented in Sect. 3 are obtained by following a similar procedure using the discrete Hamilton's principle. Additional details in this development can be found in (Lee et al. 2007).

2.1 Inertial coordinates

The configuration space of a rigid body is $\mathrm{SE}(3) = \mathbb{R}^3 \circledS \mathrm{SO}(3)$, where SO(3) denotes the group of 3×3 orthogonal matrices with unit determinant, and $\circledS$ represents a semi-direct product. We derive continuous equations of motion for n rigid bodies. We define an inertial frame and a body-fixed frame for each body, and assume that the origin of the ith body-fixed frame is located at the center of mass of the ith body.

For the ith body, the position of the center of mass in the inertial frame, and the attitude, which is a rotation matrix from the body-fixed frame to the inertial frame, are represented by $(x_i, R_i) \in \mathrm{SE}(3)$. The translational velocity in the inertial frame and the angular velocity in the body-fixed frame are represented by $v_i, \Omega_i \in \mathbb{R}^3$. The subscript i denotes the ith rigid body. The kinematic equations are given by

$$\dot{x}_i = v_i \tag{1}$$

$$\dot{R}_i = R_i S(\Omega_i), \tag{2}$$

where $S(\cdot) : \mathbb{R}^3 \mapsto \mathfrak{so}(3)$ is the isomorphism between the Lie algebra $\mathfrak{so}(3)$, which represents 3×3 skew-symmetric matrices, and $\mathbb{R}^3$ defined by: $S(x)y = x \times y$ for any $x, y \in \mathbb{R}^3$. The mass and the moment of inertia matrix of the ith body is denoted by $m_i \in \mathbb{R}$ and $J_i \in \mathbb{R}^{3\times 3}$, respectively. We construct a nonstandard moment of inertia matrix $J_{d_i} \in \mathbb{R}^{3\times 3}$ by

$$J_{d_i} = \int_{\mathcal{B}_i} \rho_i \rho_i^T \, dm_i, \tag{3}$$

where $\rho_i \in \mathbb{R}^3$ is the position of a mass element of the ith body in its body-fixed frame. It can be shown that the standard moment of inertia matrix $J_i = \int_{\mathcal{B}_i} S(\rho_i)^T S(\rho_i) dm_i \in \mathbb{R}^{3\times 3}$ is related to the nonstandard moment of inertia matrix by the following properties.

$$J_i = \mathrm{tr}\big[J_{d_i}\big]\, I_{3\times 3} - J_{d_i}, \tag{4}$$

$$S(J_i\Omega_i) = S(\Omega_i)J_{d_i} + J_{d_i}S(\Omega_i)\,, \tag{5}$$

for any $\Omega_i \in \mathbb{R}^3$. Conversely, one can obtain the nonstandard moment of inertia from the standard momentum of inertia from the following relation,

$$J_{d_i} = \frac{1}{2}\mathrm{tr}[J_i]\, I_{3\times 3} - J_i\,. \tag{6}$$

The linear momentum in the inertial frame and the angular momentum in the body-fixed frame are denoted by $\gamma_i = m_i v_i$ and $\Pi_i = J_i \Omega_i \in \mathbb{R}^3$, respectively, for the ith body.

The procedure for deriving the continuous equations of motion is shown in Fig. 1. For the given configuration space, we find an expression for the Lagrangian and the action integral. Hamilton's principle, which involves taking the variation of the action integral, yields the Euler–Lagrange equation. The Legendre transformation gives Hamilton's equation, which is equivalent to the Euler–Lagrange equation.

Lagrangian: Given $(x_i, R_i) \in \mathrm{SE}(3)$, the inertial position of a mass element of the ith body is given by $x_i + R_i\rho_i$, where $\rho_i \in \mathbb{R}^3$ denotes the position of the mass element in the body-fixed frame. Then, the kinetic energy of the ith body $\mathcal{B}_i$ can be written as

$$T_i = \tfrac{1}{2} \int_{\mathcal{B}_i} \|\dot{x}_i + \dot{R}_i\rho_i\|^2 \, dm_i.$$

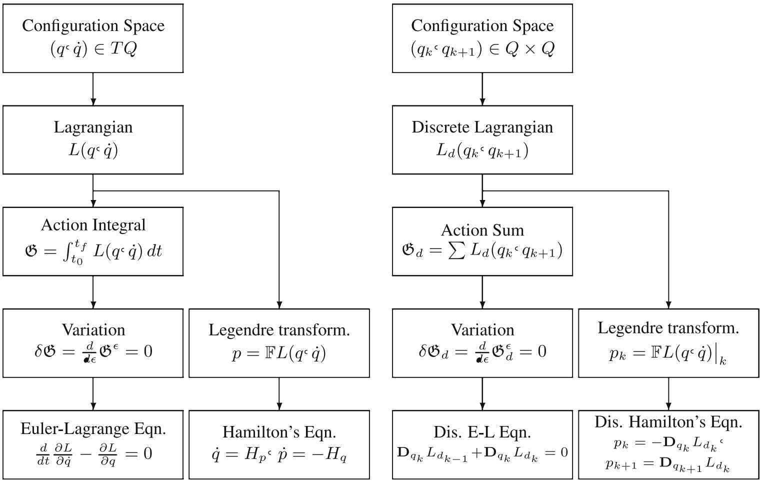


Fig. 1 Procedures to derive continuous and discrete equations of motion (Lee et al. 2007)

Using the fact that $\int_{\mathcal{B}_i} \rho_i dm_i = 0$ and (2), the kinetic energy T_i can be rewritten in terms of the nonstandard moment of inertia matrix as

$$\begin{aligned} T_i(\dot{x}_i, \Omega_i) &= \frac{1}{2}\int_{\mathcal{B}_i} \|\dot{x}_i\|^2 + \|S(\Omega_i)\rho_i\|^2\, dm_i, \\ &= \frac{1}{2} m_i \|\dot{x}_i\|^2 + \frac{1}{2}\mathrm{tr}\Big[S(\Omega_i) J_{d_i} S(\Omega_i)^T\Big]. \end{aligned} \tag{7}$$

The gravitational potential energy $U : \mathrm{SE}(3)^n \mapsto \mathbb{R}$ is given by

$$U(x_1, \ldots, x_n, R_1, \ldots, R_n) = -\frac{1}{2}\sum_{\substack{i,j=1 \\ i \neq j}}^{n} \int_{\mathcal{B}_i}\int_{\mathcal{B}_j} \frac{G dm_i dm_j}{\|x_i + R_i\rho_i - x_j - R_j\rho_j\|}, \tag{8}$$

where G is the universal gravitational constant.

Then, the Lagrangian for n rigid bodies, $L : \mathrm{TSE}(3)^n \mapsto \mathbb{R}$, is given by

$$\begin{aligned} L(x_1, \dot{x}_1, R_1, \Omega_1, \ldots, x_n, \dot{x}_n, R_n, \Omega_n) = &\sum_{i=1}^{n} \frac{1}{2} m_i \|\dot{x}_i\|^2 + \frac{1}{2}\mathrm{tr}\Big[S(\Omega_i) J_{d_i} S(\Omega_i)^T\Big] \\ &- U(x_1, \ldots, x_n, R_1 \ldots R_n). \end{aligned} \tag{9}$$

Variations of variables: Since the configuration space is $\mathrm{SE}(3)^n$, the variations should be carefully chosen so as to respect the geometry of the configuration space. The variations of $x_i, \dot{x}_i$ are trivial, namely

$$x_i^\epsilon = x_i + \epsilon\delta x_i + \mathcal{O}(\epsilon^2), \tag{10}$$

$$\dot{x}_i^\epsilon = \dot{x}_i + \epsilon\delta\dot{x}_i + \mathcal{O}(\epsilon^2), \tag{11}$$

where $\delta x_i, \delta\dot{x}_i \in \mathbb{R}^3$ are infinitesimal variations that vanish at the initial time t_0 and at the final time t_f. The infinitesimal variation of a rotation matrix R_i can be expressed in terms of a Lie algebra element $\eta_i \in \mathfrak{so}(3)$ and the exponential map as

$$\delta R_i = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} R_i \exp \epsilon\eta_i = R_i\eta_i, \tag{12}$$

where η_i vanish at the initial time t_0 and at the final time t_f. The infinitesimal variation of Ω_i can be computed from (2) and (12) to be

$$\begin{aligned} S(\delta\Omega_i) &= \frac{d}{d\epsilon}\bigg|_{\epsilon=0} R_i^{\epsilon\,T}\dot{R}_i^{\epsilon} = \delta R_i^T \dot{R}_i + R_i^T \delta\dot{R}_i, \\ &= -\eta_i S(\Omega_i) + S(\Omega_i)\eta_i + \dot{\eta}_i. \end{aligned} \tag{13}$$

Hamilton's principle: The action integral is defined to be

$$\mathfrak{G} = \int_{t_0}^{t_f} L(x_1, \dot{x}_1, R_1, \Omega_1, \ldots, x_n, \dot{x}_n, R_n, \Omega_n)\, \mathrm{d}t. \tag{14}$$

Using the variational expression (10)–(13), the variation of the action integral can be written as

$$\delta\mathfrak{G} = \sum_{i=1}^{n} \int_{t_0}^{t_f} m_i \dot{x}_i^T \delta\dot{x}_i - \frac{\partial U}{\partial x_i}^T \delta x_i + \tfrac{1}{2}\mathrm{tr}\Big[-\dot{\eta}_i S(J_i\Omega_i) + \eta_i \Big\{S(\Omega_i \times J_i\Omega_i) + 2R_i^T \tfrac{\partial U}{\partial R_i}\Big\}\Big]\, \mathrm{d}t,$$

where $\frac{\partial U}{\partial R_i} \in \mathbb{R}^{3\times 3}$ is determined by the relationship, $[\frac{\partial U}{\partial R_i}]_{p,q} = \frac{\partial U}{\partial [R_i]_{p,q}}$. Here $[A]_{p,q}$ denotes the (p,q)th element of a matrix A. Using integration by parts and the fact that δx_i and η_i vanish at t_0 and t_f, $\delta\mathfrak{G}$ is given by

$$\begin{aligned} \delta\mathfrak{G} = \sum_{i=1}^{n} \int_{t_0}^{t_f} & -\delta x_i^T \left\{ m_i \ddot{x}_i + \frac{\partial U}{\partial x_i} \right\} \\ & + \frac{1}{2}\mathrm{tr}\left[\eta_i \left\{ S(J_i\dot{\Omega}_i + \Omega_i \times J_i\Omega_i) + 2R_i^T \frac{\partial U}{\partial R_i} \right\} \right] \mathrm{d}t. \end{aligned} \tag{15}$$

From Hamilton's principle, $\delta\mathfrak{G}$ should be zero for all possible variations $\delta x_i \in \mathbb{R}^3$ and $\eta_i \in \mathfrak{so}(3)$. Therefore, the expression in the first brace should be zero, and the expression in the second brace should be symmetric, since η_i is skew-symmetric. Then, we obtain the continuous equations of motion as

$$\begin{aligned} m_i \ddot{x}_i &= -\frac{\partial U}{\partial x_i}, \\ S(J_i\dot{\Omega}_i + \Omega_i \times J_i\Omega_i) &= \frac{\partial U}{\partial R_i}^T R - R_i^T \frac{\partial U}{\partial R_i}. \end{aligned}$$

Note that the right hand side expression in the second equation is skew-symmetric. The moment due to the gravitational potential on the ith body, $M_i \in \mathbb{R}^3$, can be expressed explicitly as the following computation shows.

$$\begin{aligned} S(M_i) &= \frac{\partial U}{\partial R_i}^T R_i - R_i^T \frac{\partial U}{\partial R_i}, \\ &= \begin{bmatrix} u_{i_1}^T & u_{i_2}^T & u_{i_2}^T \end{bmatrix} \begin{bmatrix} r_{i_1} \\ r_{i_2} \\ r_{i_3} \end{bmatrix} - \begin{bmatrix} r_{i_1}^T & r_{i_2}^T & r_{i_3}^T \end{bmatrix} \begin{bmatrix} u_{i_1} \\ u_{i_2} \\ u_{i_3} \end{bmatrix}, \\ &= \left(u_{i_1}^T r_{i_1} - r_{i_1}^T u_{i_1}\right) + \left(u_{i_2}^T r_{i_2} - r_{i_2}^T u_{i_2}\right) + \left(u_{i_3}^T r_{i_3} - r_{i_3}^T u_{i_3}\right), \end{aligned}$$

where $r_{i_p}, u_{i_p} \in \mathbb{R}^{1\times 3}$ are the pth row vectors of R_i and $\frac{\partial U}{\partial R_i}$, respectively. Since $S(x\times y) = yx^T - xy^T$ for any column vectors $x, y \in \mathbb{R}^3$, we obtain

$$M_i = r_{i_1} \times u_{i_1} + r_{i_2} \times u_{i_2} + r_{i_3} \times u_{i_3}. \tag{16}$$

Equations of motion: In summary, *the continuous equations of motion for the full body problem, in Lagrangian form,* can be written for bodies $i \in (1, 2, \cdots, n)$ as

$$\dot{v}_i = -\frac{1}{m_i}\frac{\partial U}{\partial x_i}, \tag{17}$$

$$J_i\dot{\Omega}_i + \Omega_i \times J_i\Omega_i = M_i, \tag{18}$$

$$\dot{x}_i = v_i, \tag{19}$$

$$\dot{R}_i = R_i S(\Omega_i). \tag{20}$$

where the gravitational moment M_i is obtained by (16). The above equations can be readily rewritten in Hamiltonian form, using the definition of the linear momentum and the angular momentum, $\gamma_i = m_i v_i$, and $\Pi_i = J_i\Omega_i$.

2.2 Relative coordinates

The motion of the full rigid bodies depends only on the relative positions and the relative attitudes of the bodies. This is a consequence of the property that the gravitational potential can be expressed in terms of only these relative variables. Physically, this is related to the fact that the total linear momentum and the total angular momentum about the mass center of the bodies are conserved. Mathematically, the Lagrangian is invariant under the lifted left action of an element of SE(3). So, it is natural to express the equations of motion in one of the body-fixed frames. In this section, the equations of motion for the full two body problem are derived in relative coordinates. This result can be readily generalized to the n body problem.

Reduction of variables: In (Maciejewski 1995), the reduction is carried out in stages, by first reducing position variables in $\mathbb{R}^3$, and then reducing attitude variables in SO(3). This is equivalent to directly reducing the position and the attitude variables in SE(3) in a single step, which is a consequence of the general theory of Lagrangian reduction by stages (Cendra et al. 2001).

We express each variable with respect to the second body-fixed frame. The reduced position and the reduced attitude variables are the relative position and the relative attitude of the first body with respect to the second body. In other words, the variables are reduced by applying the inverse of $(x_2, R_2) \in \mathrm{SE}(3)$, given by $(-R_2^T x_2, R_2^T) \in \mathrm{SE}(3)$, to each variable, which can be written using homogeneous coordinates:

$$\begin{bmatrix} R_2^T & -R_2^T x_2 \\ 0 & 1 \end{bmatrix}\left(\begin{bmatrix} R_1 & x_1 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} R_2 & x_2 \\ 0 & 1 \end{bmatrix}\right) = \left(\begin{bmatrix} R_2^T R_1 & R_2^T(x_1 - x_2) \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} R_2^T R_2 & R_2^T(x_2 - x_2) \\ 0 & 1 \end{bmatrix}\right),$$

$$= \left(\begin{bmatrix} R_2^T R_1 & R_2^T(x_1 - x_2) \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} I_{3\times 3} & 0 \\ 0 & 1 \end{bmatrix}\right). \tag{21}$$

This motivates the definition of the reduced variables as

$$X = R_2^T(x_1 - x_2), \tag{22}$$

$$R = R_2^T R_1, \tag{23}$$

where $X \in \mathbb{R}^3$ is the relative position of the first body with respect to the second body expressed in the second body-fixed frame, and $R \in \mathrm{SO}(3)$ is the relative attitude of the first body with respect to the second body. The corresponding linear and angular velocities are also defined as

$$V = R_2^T(\dot{x}_1 - \dot{x}_2), \tag{24}$$

$$\Omega = R\Omega_1, \tag{25}$$

where $V \in \mathbb{R}^3$ represents the relative velocity of the first body with respect to the second body in the second body-fixed frame, and $\Omega \in \mathbb{R}^3$ is the angular velocity of the first body expressed in the second body-fixed frame. Here, the capital letters denote variables expressed in the second body-fixed frame. For convenience, we denote the inertial position and the inertial velocity of the second body, expressed in the second body-fixed frame by $X_2, V_2 \in \mathbb{R}^3$:

$$X_2 = R_2^T x_2, \tag{26}$$

$$V_2 = R_2^T \dot{x}_2. \tag{27}$$

The moment of inertia matrices of the first body are expressed with respect to the second body-fixed frame. We define $J_R = RJ_1R^T, J_{d_R} = RJ_{d_1}R^T \in \mathbb{R}^{3\times3}$. Note that J_R and J_{d_R} are not constant. It can be shown that J_{d_R} also satisfies a property similar to (5), namely

$$S(J_R\Omega) = S(\Omega)J_{d_R} + J_{d_R}S(\Omega) \tag{28}$$

for any $\Omega \in \mathbb{R}^3$. Define the linear momenta $\Gamma, \gamma_2 \in \mathbb{R}^3$, and the angular momenta $\Pi, \Pi_2 \in \mathbb{R}^3$ as

$$\Gamma = mV, \tag{29}$$

$$\gamma_2 = mv_2, \tag{30}$$

$$\Pi = J_R\Omega = RJ_1\Omega_1, \tag{31}$$

$$\Pi_2 = J_2\Omega_2. \tag{32}$$

The equations of motion in relative coordinates are derived in the same way used to derive the equations in the inertial frame. Here, the Lagrangian is expressed in terms of the reduced variables, and the expressions for the reduced variations are derived.

Reduced Lagrangian: The reduced Lagrangian l is obtained by expressing the original Lagrangian (9) for two bodies in terms of the reduced variables. The kinetic energy is given by

$$T_1 + T_2 = \frac{1}{2}m_1 \|V + V_2\|^2 + \frac{1}{2}m_2 \|V_2\|^2 + \frac{1}{2}\mathrm{tr}\left[S(\Omega)J_{d_R}S(\Omega)^T\right] + \frac{1}{2}\mathrm{tr}\left[S(\Omega_2)J_{d_2}S(\Omega_2)^T\right],$$

The gravitational potential can be written as a function of the relative variables only. By applying the inverse of $(R_2, x_2) \in \mathrm{SE}(3)$ as given in (21), we obtain

$$\begin{aligned} U(x_1, x_2, R_1, R_2) &= U(R_2^T(x_1 - x_2), 0, R_2^T R_1, I_{3\times3}), \\ &= -\int_{\mathcal{B}_1}\int_{\mathcal{B}_2} \frac{Gdm_1dm_2}{\|X + R\rho_1 - \rho_2\|}, \\ &\triangleq U(X, R). \end{aligned}$$

Here, we abuse notation slightly by using the same letter U to denote the gravitational potential as a function of the relative variables. Then, the reduced Lagrangian l is given by

$$\begin{aligned} l(R,X,\Omega,V,\Omega_2,V_2) = \; & \frac{1}{2}m_1\|V+V_2\|^2+\frac{1}{2}m_2\|V_2\|^2 \\ & +\frac{1}{2}\mathrm{tr}\Big[S(\Omega)J_{d_R}S(\Omega)^T\Big]+\frac{1}{2}\mathrm{tr}\Big[S(\Omega_2)J_{d_2}S(\Omega_2)^T\Big] \\ & -U(X,R). \end{aligned} \tag{33}$$

Variations of reduced variables: The variations of the reduced variables must be restricted to those that arise from variations of the original variables. For example, the variation of the relative attitude R is given by

$$\delta R = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} R_2^{\epsilon T} R_1^{\epsilon} = \delta R_2^T R_1 + R_2^T \delta R_1.$$

Substituting (12) into the above equation,

$$\begin{aligned} \delta R &= -\eta_2 R_2^T R_1 + R_2^T R_1 \eta_1, \\ &= -\eta_2 R + \eta R, \end{aligned}$$

where a reduced variation $\eta \in \mathfrak{so}(3)$ is defined as $\eta = R\eta_1 R^T$. The variations of other reduced variables can be obtained in a similar way:

$$\delta R = \eta R - \eta_2 R, \tag{34}$$

$$\delta X = \chi - \eta_2 X, \tag{35}$$

$$S(\delta\Omega) = \dot{\eta} - S(\Omega)\eta + \eta S(\Omega) + S(\Omega)\eta_2 - \eta_2 S(\Omega) + S(\Omega_2)\eta - \eta S(\Omega_2), \tag{36}$$

$$\delta V = \dot{\chi} + S(\Omega_2)\chi - \eta_2 V, \tag{37}$$

$$S(\delta\Omega_2) = \dot{\eta}_2 + S(\Omega_2)\eta_2 - \eta_2 S(\Omega_2), \tag{38}$$

$$\delta V_2 = \dot{\chi}_2 + S(\Omega_2)\chi_2 - \eta_2 V_2, \tag{39}$$

where $\chi, \chi_2 \in \mathbb{R}^3$ and $\eta, \eta_2 \in \mathfrak{so}(3)$ are variations that vanish at the end points. These Lie group variations are the key elements required to obtain the equations of motion in relative coordinates.

Reduced equations of motion: The reduced equations of motion can be computed from the reduced Lagrangian using the reduced Hamilton's principle. By taking the variation of the reduced Lagrangian (33) using the constrained variations given by (34) through (39), we obtain the variation of the action integral similar to (15). The reduced Hamilton's principle yields the following *continuous equations of relative motion for the full two body problem, in Lagrangian form*

$$\dot{V} + \Omega_2 \times V = -\frac{1}{m}\frac{\partial U}{\partial X}, \tag{40}$$

$$(\dot{J_R\Omega}) + \Omega_2 \times J_R\Omega = -M, \tag{41}$$

$$J_2\dot{\Omega}_2 + \Omega_2 \times J_2\Omega_2 = X \times \frac{\partial U}{\partial X} + M, \tag{42}$$

$$\dot{X} + \Omega_2 \times X = V, \tag{43}$$

$$\dot{R} = S(\Omega)R - S(\Omega_2)R, \tag{44}$$

where $m = \frac{m_1 m_2}{m_1+m_2} \in \mathbb{R}$, and the moment due to the gravity potential $M \in \mathbb{R}^3$ is obtained by

$$M = r_1 \times u_{r_1} + r_2 \times u_{r_2} + r_3 \times u_{r_3}, \tag{45}$$

where $r_p, u_{r_p} \in \mathbb{R}^3$ are the pth column vectors of R and $\frac{\partial U}{\partial R}$, respectively. The following equations can be used for reconstruction of the motion of the second body in the inertial frame:

$$\dot{v}_2 = \frac{1}{m_2} R_2 \frac{\partial U}{\partial X}, \tag{46}$$

$$\dot{x}_2 = v_2, \tag{47}$$

$$\dot{R}_2 = R_2 S(\Omega_2). \tag{48}$$

These equations are equivalent to those given by (Maciejewski 1995), although he omitted the reconstruction equations. Equations (40) though (48) give a complete set of equations for the reduced dynamics and reconstruction. Furthermore, they are derived systematically in the context of geometric mechanics using proper variational formulas given in (34) through (39). The above equations can be readily rewritten in Hamiltonian form using (29)–(32).

3 Lie group variational integrators

General purpose numerical integration methods, including the popular explicit (non-symplectic) Runge-Kutta methods, fail to preserve the geometric characteristics of the full body problem. Integration formulas are obtained by approximating the continuous equations of motion by directly discretizing them with respect to time. With each integration step, the updates involve additive operations, so that the underlying Lie group structure is not necessarily preserved as time progresses. This is caused by the fact that the Euclidean Lie group is not closed under addition. For example, if we use a Runge–Kutta method for numerical integration of (44), then the rotation matrices inevitably drift from the orthogonal rotation group SO(3); the quantity $R^T R$ drifts from the identity matrix. Then, the attitudes of the rigid bodies are not determined accurately, resulting in significant errors in computation of the gravitational forces and moments that depend on the attitude, and consequently errors in the entire simulation. It is often proposed to parameterize (44) by Euler angles or unit quaternions. However, Euler angles are not global expressions of the attitude since they have associated singularities. Unit quaternions do not exhibit singularities, but they are constrained to lie on the unit three-sphere $\mathbb{S}^3$; general purpose numerical integration methods do not preserve the unit length constraint. Therefore, quaternions lead to the same numerical drift problem. Re-normalizing the quaternion vector at each step destroys the conservation properties. Furthermore, unit quaternions double cover SO(3), so that there are inevitable ambiguities in expressing the attitude.

One might instead attempt to apply a symplectic Runge–Kutta algorithm to a rotation matrix based formulation of the problem. But even if it were possible to reproject the numerical solution onto SO(3) while preserving the energy, momentum, and symplectic properties, this would still introduce a drift in the energy. This is because the symplectic integrator does not exactly preserve the energy; instead, the numerical solution evolves on the isoenergy surface of a modified Hamiltonian

(Hairer et al. 2006), which is close to the isoenergy surface of the original Hamiltonian. This is why symplectic integrators exhibit bounded energy fluctuations, as the two isoenergy surfaces are always close, but do not coincide. Since explicit expressions for the modified Hamiltonian do not exist, the reprojection invariably changes the modified Hamiltonian associated with the discrete flow, which in turn introduces a drift in the energy if reprojection is performed repeatedly. Indeed, it was shown in (Ge and Marsden 1988) that a fixed time-step numerical algorithm cannot simultaneously preserve the energy, momentum, and symplecticity, unless it samples the exact trajectory of the system. It is however possible to construct variable time-step methods that are symplectic-energy-momentum preserving integrators (Kane et al. 1999).

In contrast, the Lie Group Variational Integrator has desirable properties such as symplecticity, momentum preservation, and good energy stability for exponentially long time periods, while simultaneously preserving the Euclidian Lie group structure without the use of local charts, reprojection, or constraints. The LGVI is obtained by discretizing Hamilton's principle as shown in Fig. 1; the velocity phase space of the continuous Lagrangian is replaced by discrete variables, and a discrete Lagrangian is chosen such that it approximates a segment of the action integral. Taking the variation of the resulting action sum, we obtain discrete equations of motion referred to as a variational integrator. Since the discrete variables are updated by Lie group operations, the group structure is preserved automatically.

In this section, we derive both a Lagrangian and Hamiltonian form of variational integrators for the full body problem in inertial and relative coordinates. The second level subscript k denotes the value of variables at $t = kh + t_0$ for an integration step size $h \in \mathbb{R}$ and an integer k. The integer N satisfies $t_f = kN + t_0$, so N is the number of time-steps of length h to go from the initial time t_0 to the final time t_f.

3.1 Inertial coordinates

Discrete Lagrangian: In continuous time, the structure of the kinematic equations (20), (44) and (48) ensure that R_i, R and R_2 evolve on SO(3) automatically. Here, we introduce a new variable $F_{i_k} \in \mathrm{SO}(3)$ defined such that $R_{i_{k+1}} = R_{i_k} F_{i_k}$, i.e.

$$F_{i_k} = R_{i_k}^T R_{i_{k+1}}. \tag{49}$$

Thus, F_{i_k} represents the relative attitude between two integration steps, and by requiring that $F_{i_k} \in \mathrm{SO}(3)$, we guarantee that R_{i_k} evolves on SO(3) automatically. This is a consequence of the fact that the Lie group is closed under the group operation of matrix multiplication.

Using the kinematic equation $\dot{R}_i = R_i S(\Omega_i)$, the skew-symmetric matrix $S(\Omega_k)$ can be approximated as

$$S(\Omega_{i_k}) = R_{i_k}^T \dot{R}_{i_k} \approx R_{i_k}^T \frac{R_{i_{k+1}} - R_{i_k}}{h} = \frac{1}{h}(F_{i_k} - I_{3\times3}). \tag{50}$$

The velocity $\dot{x}_{i_k}$ can be approximated simply by $(x_{i_{k+1}} - x_{i_k})/h$. Using these approximations of the angular and linear velocity, the kinetic energy of the ith body given in (7) can be approximated as

$$T_i(\dot{x}_i, \Omega_i) \approx T_i\left(\frac{1}{h}(x_{i_{k+1}} - x_{i_k}), \frac{1}{h}(F_{i_k} - I_{3\times3})\right),$$
$$= \frac{1}{2h^2} m_i \left\| x_{i_{k+1}} - x_{i_k} \right\|^2 + \frac{1}{2h^2}\mathrm{tr}\Big[(F_{i_k} - I_{3\times3})J_{d_i}(F_{i_k} - I_{3\times3})^T\Big],$$
$$= \frac{1}{2h^2} m_i \left\| x_{i_{k+1}} - x_{i_k} \right\|^2 + \frac{1}{h^2}\mathrm{tr}\big[(I_{3\times3} - F_{i_k})J_{d_i}\big].$$

A discrete Lagrangian $L_d : \mathrm{SE}(3)^n \times \mathrm{SE}(3)^n \mapsto \mathbb{R}$ is constructed such that it approximates a segment of the action integral (14),

$$L_d = \sum_{i=1}^{n} \frac{1}{2h} m_i \left\| x_{i_{k+1}} - x_{i_k} \right\|^2 + \frac{1}{h}\mathrm{tr}\big[(I_{3\times3} - F_{i_k})J_{d_i}\big]$$
$$-\frac{h}{2}U(x_{1_k}, \ldots, R_{n_k}) - \frac{h}{2}U(x_{1_{k+1}}, \ldots, R_{n_{k+1}}). \tag{51}$$

This discrete Lagrangian is self-adjoint (Hairer et al. 2006), and self-adjoint numerical integration methods have even order, so we are guaranteed that the resulting integration method is at least second-order accurate.

Variations of discrete variables: The variations of the discrete variables are chosen to respect the geometry of the configuration space SE(3). The variation of x_{i_k} is given by

$$x_{i_k}^{\epsilon} = x_{i_k} + \epsilon\delta x_{i_k} + \mathcal{O}(\epsilon^2),$$

where $\delta x_{i_k} \in \mathbb{R}^3$ and vanishes at $k = 0$ and $k = N$. The variation of R_{i_k} is given by

$$\delta R_{i_k} = R_{i_k}\eta_{i_k}, \tag{52}$$

where $\eta_{i_k} \in \mathfrak{so}(3)$ is a variation represented by a skew-symmetric matrix and vanishes at $k = 0$ and $k = N$. The variation of F_{i_k} can be computed from the definition $F_{i_k} = R_{i_k}^T R_{i_{k+1}}$ to give

$$\delta F_{i_k} = \delta R_{i_k}^T R_{i_{k+1}} + R_{i_k}^T \delta R_{i_{k+1}},$$
$$= -\eta_{i_k} R_{i_k}^T R_{i_{k+1}} + R_{i_k}^T R_{i_{k+1}} \eta_{i_{k+1}},$$
$$= -\eta_{i_k} F_{i_k} + F_{i_k}\eta_{i_{k+1}}. \tag{53}$$

Discrete Hamilton's principle: To obtain the discrete equations of motion in Lagrangian form, we compute the variation of the discrete Lagrangian from (52) and (53) to give

$$\delta L_d = \sum_{i=1}^{n} \frac{1}{h} m_i (x_{i_{k+1}} - x_{i_k})^T(\delta x_{i_{k+1}} - \delta x_{i_k}) + \frac{1}{h}\mathrm{tr}\big[\big(\eta_{i_k}F_{i_k} - F_{i_k}\eta_{i_{k+1}}\big)J_{d_i}\big]$$
$$-\frac{h}{2}\left(\frac{\partial U_k}{\partial x_{i_k}}^T \delta x_{i_k} + \frac{\partial U_{k+1}}{\partial x_{i_{k+1}}}^T \delta x_{i_{k+1}}\right) + \frac{h}{2}\mathrm{tr}\left[\eta_{i_k} R_{i_k}^T \frac{\partial U_k}{\partial R_{i_k}} + \eta_{i_{k+1}} R_{i_{k+1}}^T \frac{\partial U_{k+1}}{\partial R_{i_{k+1}}}\right], \tag{54}$$

where $U_k = U(x_{1_k}, \ldots, R_{n_k})$ denotes the value of the potential at $t = kh + t_0$.

Define the action sum as

$$\mathfrak{G}_d = \sum_{k=0}^{N-1} L_d(x_{1_k}, x_{1_{k+1}}, R_{1_k}, F_{1_k}, \ldots, x_{n_k}, x_{n_{k+1}}, R_{n_k}, F_{n_k}). \tag{55}$$

The discrete action sum $\mathfrak{G}_d$ approximates the action integral (14), because the discrete Lagrangian approximates a segment of the action integral. Substituting (54) into (55), the variation of the action sum is given by

$$\delta\mathfrak{G}_d = \sum_{k=0}^{N-1}\sum_{i=1}^{n} \delta x_{i_{k+1}}^T \left\{\frac{1}{h}m_i(x_{i_{k+1}} - x_{i_k}) - \frac{h}{2}\frac{\partial U_{k+1}}{\partial x_{i_{k+1}}}\right\} + \delta x_{i_k}^T \left\{-\frac{1}{h}m_i(x_{i_{k+1}} - x_{i_k}) - \frac{h}{2}\frac{\partial U_k}{\partial x_{i_k}}\right\}$$
$$+\mathrm{tr}\left[\eta_{i_{k+1}}\left\{-\frac{1}{h}J_{d_i}F_{i_k} + \frac{h}{2}R_{i_{k+1}}^T\frac{\partial U_{k+1}}{\partial R_{i_{k+1}}}\right\}\right] + \mathrm{tr}\left[\eta_{i_k}\left\{\frac{1}{h}F_{i_k}J_{d_i} + \frac{h}{2}R_{i_k}^T\frac{\partial U_k}{\partial R_{i_k}}\right\}\right].$$

Using the fact that δx_{i_k} and η_{i_k} vanish at $k = 0$ and $k = N$, we can reindex the summation, which is the discrete analogue of integration by parts, to yield

$$\delta\mathfrak{G}_d = \sum_{k=1}^{N-1}\sum_{i=1}^{n} -\delta x_{i_k}\left\{\frac{1}{h}m_i\left(x_{i_{k+1}} - 2x_{i_k} + x_{i_{k-1}}\right) + h\frac{\partial U_k}{\partial x_{i_k}}\right\}$$
$$+\mathrm{tr}\left[\eta_{i_k}\left\{\frac{1}{h}\left(F_{i_k}J_{d_i} - J_{d_i}F_{i_{k-1}}\right) + hR_{i_k}^T\frac{\partial U_k}{\partial R_{i_k}}\right\}\right].$$

Hamilton's principle states that $\delta\mathfrak{G}_d$ should be zero for all possible variations $\delta x_{i_k} \in \mathbb{R}^3$ and $\eta_{i_k} \in \mathfrak{so}(3)$ that vanish at the endpoints. Therefore, the expression in the first brace should be zero, and since η_{i_k} is skew-symmetric, the expression in the second brace should be symmetric.

Discrete equations of motion: We obtain *the discrete equations of motion for the full body problem, in Lagrangian form,* for bodies $i \in (1, 2, \cdots, n)$ as

$$\frac{1}{h}\left(x_{i_{k+1}} - 2x_{i_k} + x_{i_{k-1}}\right) = -h\frac{\partial U_k}{\partial x_{i_k}}, \tag{56}$$

$$\frac{1}{h}\left(F_{i_{k+1}}J_{d_i} - J_{d_i}F_{i_{k+1}}^T - J_{d_i}F_{i_k} + F_{i_k}^TJ_{d_i}\right) = hS(M_{i_{k+1}}), \tag{57}$$

$$R_{i_{k+1}} = R_{i_k}F_{i_k}, \tag{58}$$

where $M_{i_k} \in \mathbb{R}^3$ is defined in (16) as

$$M_{i_k} = r_{i_1} \times u_{i_1} + r_{i_2} \times u_{i_2} + r_{i_3} \times u_{i_3}, \tag{59}$$

where $r_{i_p}, u_{i_p} \in \mathbb{R}^{1\times 3}$ are pth row vectors of R_{i_k} and $\frac{\partial U_k}{\partial R_{i_k}}$, respectively. Given initial conditions $(x_{i_0}, R_{i_0}, x_{i_1}, R_{i_1})$, we can obtain x_{i_2} from (56). Then, F_{i_0} is computed from (58), and F_{i_1} can be obtained by solving the implicit equation (57). Finally, R_{i_2} is found from (58). This yields an update map $(x_{i_0}, R_{i_0}, x_{i_1}, R_{i_1}) \mapsto (x_{i_1}, R_{i_1}, x_{i_2}, R_{i_2})$, and this process can be repeated.

As discussed above, Eqs. (56) through (58) defines a discrete Lagrangian map that updates x_{i_k} and R_{i_k}. The discrete Legendre transformation relates the configuration variables x_{i_k}, R_{i_k} and the corresponding momenta γ_{i_k}, Π_{i_k}. This induces a discrete Hamiltonian map that is equivalent to the discrete Lagrangian map. The detailed development of the discrete Legendre transformation can be found in (Lee et al. 2007); here we summarize the result.

The discrete equations of motion for the full body problem, in Hamiltonian form, can be written for bodies $i \in (1, 2, \cdots, n)$ as

$$x_{i_{k+1}} = x_{i_k} + \frac{h}{m_i}\gamma_{i_k} - \frac{h^2}{2m_i}\frac{\partial U_k}{\partial x_{i_k}}, \tag{60}$$

$$\gamma_{i_{k+1}} = \gamma_{i_k} - \frac{h}{2}\frac{\partial U_k}{\partial x_{i_k}} - \frac{h}{2}\frac{\partial U_{k+1}}{\partial x_{i_{k+1}}}, \tag{61}$$

$$hS(\Pi_{i_k} + \frac{h}{2}M_{i_k}) = F_{i_k}J_{d_i} - J_{d_i}F_{i_k}^T, \tag{62}$$

$$\Pi_{i_{k+1}} = F_{i_k}^T\Pi_{i_k} + \frac{h}{2}F_{i_k}^T M_{i_k} + \frac{h}{2}M_{i_{k+1}}., \tag{63}$$

$$R_{i_{k+1}} = R_{i_k}F_{i_k}. \tag{64}$$

Given $(x_{i_0}, \gamma_{i_0}, R_{i_0}, \Pi_{i_0})$, we can find x_{i_1} from (60). Solving the implicit equation (62) yields F_{i_0}, and R_{i_1} is computed from (64). Then, (61) and (63) gives γ_{i_1}, and Π_{i_1}. This defines the discrete Hamiltonian map, $(x_{i_0}, \gamma_{i_0}, R_{i_0}, \Pi_{i_0}) \mapsto (x_{i_1}, \gamma_{i_1}, R_{i_1}, \Pi_{i_1})$, and this process can be repeated.

3.2 Relative coordinates

In this section, we derive the variational integrator for the full two body problem in relative coordinates by expressing the discrete Lagrangian in relative coordinates, and then computing the constrained variations of the discrete reduced variables. This result can be readily generalized to n bodies. A more intrinsic development of discrete Routh reduction can be found in Jalnapurkar et al. (2006).

Reduction of discrete variables: The discrete reduced variables are defined in the same way as the continuous reduced variables, which are given in (22) through (32). We introduce $F_k \in \mathrm{SO}(3)$ such that $R_{k+1} = R_{2_{k+1}}^T R_{1_{k+1}} = F_{2_k}^T F_k R_k$, i.e.

$$F_k = R_k F_{1_k} R_k^T. \tag{65}$$

Discrete reduced Lagrangian: The discrete reduced Lagrangian is obtained by expressing the original discrete Lagrangian given in (51) in terms of the discrete reduced variables.

From the definition of the discrete reduced variables given in (22) and (26), we have

$$\begin{aligned} x_{1_{k+1}} - x_{1_k} &= R_{2_{k+1}}(X_{k+1} + X_{2_{k+1}}) - R_{2_k}(X_k + X_{2_k}), \\ &= R_{2_k}\left\{F_{2_k}(X_{k+1} + X_{2_{k+1}}) - (X_k + X_{2_k})\right\}, \end{aligned} \tag{66}$$

$$x_{2_{k+1}} - x_{2_k} = R_{2_k}\left\{F_{2_k}X_{2_{k+1}} - X_{2_k}\right\}. \tag{67}$$

From (50), $S(\Omega_{1_k})$ and $S(\Omega_{2_k})$ are expressed as

$$S(\Omega_{1_k}) = \frac{1}{h}\left(F_{1_k} - I_{3\times3}\right) = \frac{1}{h}R_k^T\left(F_k - I_{3\times3}\right)R_k, \tag{68}$$

$$S(\Omega_{2_k}) = \frac{1}{h}\left(F_{2_k} - I_{3\times3}\right). \tag{69}$$

Substituting (66) through (69) into (51), we obtain the discrete reduced Lagrangian.

$$
\begin{aligned}
l_{d_k} &= l_d(X_k, X_{k+1}, X_{2_k}, X_{2_{k+1}}, R_k, F_k, F_{2_k}) \\
&= \frac{1}{2h} m_1 \left\| F_{2_k}(X_{k+1} + X_{2_{k+1}}) - (X_k + X_{2_k}) \right\|^2 + \frac{1}{2h} m_2 \left\| F_{2_k} X_{2_{k+1}} - X_{2_k} \right\|^2 \\
&\quad + \frac{1}{h}\mathrm{tr}\big[(I_{3\times 3} - F_k) J_{dR_k}\big] + \frac{1}{h}\mathrm{tr}\big[(I_{3\times 3} - F_{2_k}) J_{d_2}\big] \\
&\quad - \frac{h}{2} U(X_k, R_k) - \frac{h}{2} U(X_{k+1}, R_{k+1}),
\end{aligned} \tag{70}
$$

where $J_{dR_k} \in \mathbb{R}^{3\times 3}$ is defined to be $J_{dR_k} = R_k J_{d_1} R_k^T$, which gives the nonstandard moment of inertia matrix of the first body with respect to the second body-fixed frame at $t = kh + t_0$.

Variations of discrete reduced variables: The variations of the discrete reduced variables can be derived from those of the original variables. The variations of R_k, X_k, and F_{2_k} are the same as those given in (34), (35), and (53), respectively. The variation of F_k is computed in a similar fashion to (53). In summary, the variations of discrete reduced variables are given by

$$\delta R_k = \eta_k R_k - \eta_{2_k} R_k, \tag{71}$$

$$\delta X_k = \chi_k - \eta_{2_k} X_k, \tag{72}$$

$$\delta F_k = -\eta_{2_k} F_k + F_{2_k} \eta_{k+1} F_{2_k}^T F_k + F_k \left(-\eta_k + \eta_{2_k}\right), \tag{73}$$

$$\delta X_{2_k} = \chi_{2_k} - \eta_{2_k} X_{2_k}, \tag{74}$$

$$\delta F_{2_k} = -\eta_{2_k} F_{2_k} + F_{2_k} \eta_{2_{k+1}}. \tag{75}$$

These Lie group variations are the main elements required to derive the variational integrator equations.

Discrete reduced equations of motion: Define the action sum in terms of the discrete reduced Lagrangian

$$\mathfrak{G}_d = \sum_{k=0}^{N-1} l_d(X_k, X_{k+1}, X_{2_k}, X_{2_{k+1}}, R_k, F_k, F_{2_k}). \tag{76}$$

Using the expressions for the reduced variations, (71)–(75), we obtain the variation of the action sum. From Hamilton's principle, it should be zero for all possible variations $\chi_k, \chi_{2_k} \in \mathbb{R}^3$ and $\eta_k, \eta_{2_k} \in \mathfrak{so}(3)$ which vanish at the endpoints.

As a result, *the discrete equations of relative motion for the full two body problem, in Lagrangian form,* are obtained as

$$F_{2_k} X_{k+1} - 2X_k + F_{2_{k-1}}^T X_{k-1} = -\frac{h^2}{m} \frac{\partial U_k}{\partial X_k}, \tag{77}$$

$$F_{k+1} J_{dR_{k+1}} - J_{dR_{k+1}} F_{k+1}^T = F_{2_k}^T \left(F_k J_{dR_k} - J_{dR_k} F_k^T\right) F_{2_k} - h^2 S(M_{k+1}), \tag{78}$$

$$
\begin{aligned}
F_{2_{k+1}} J_{d_2} - J_{d_2} F_{2_{k+1}}^T &= F_{2_k}^T \left(F_{2_k} J_{d_2} - J_{d_2} F_{2_k}^T\right) F_{2_k} \\
&\quad + h^2 X_{k+1} \times \frac{\partial U}{\partial X_{k+1}} + h^2 S(M_{k+1}),
\end{aligned} \tag{79}
$$

$$R_{k+1} = F_{2_k}^T F_k R_k, \tag{80}$$

$$R_{2_{k+1}} = R_{2_k} F_{2_k}. \tag{81}$$

It is natural to express the equations of motion for the second body in the inertial frame.

$$x2_{k+1} - 2x2_k + x2_{k-1} = \frac{h^2}{m_2} R_k \frac{\partial U_k}{\partial X_k}. \tag{82}$$

Given $(X_0, R_0, R2_0, X_1, R_1, R2_1)$, we can determine F_0 and $F2_0$ from (80) and (81). Solving the implicit equations (78) and (79) gives F_1 and $F2_1$. Then X_2, R_2 and $R2_2$ are found from (77), (80) and (81), respectively. This yields the discrete Lagrangian map $(X_0, R_0, R2_0, X_1, R_1, R2_1) \mapsto (X_1, R_1, R2_1, X_2, R_2, R2_2)$ and this process can be repeated. We can separately reconstruct $x2_k$ using (82).

Alternatively, once we have obtained F_0 and $F2_0$ from (80) and (81), we can view Eqs. (78), (79), (77) and (80) as defining an implicit update map $(X_0, R_0, F_0, F2_0, X_1) \mapsto (X_1, R_1, F_1, F2_1, X_2)$. As a post-processing step, $R2_k$ and $x2_k$ can be reconstructed using (81) and (82), respectively.

The discrete Legendre transformation yields *the discrete equations of relative motion for the full two body problem, in Hamiltonian form,*

$$X_{k+1} = F2_k^T \left(X_k + h\frac{\Gamma_k}{m} - \frac{h^2}{2m}\frac{\partial U_k}{\partial X_k} \right), \tag{83}$$

$$\Gamma_{k+1} = F2_k^T \left(\Gamma_k - \frac{h}{2}\frac{\partial U_k}{\partial X_k} \right) - \frac{h}{2}\frac{\partial U_{k+1}}{\partial X_{k+1}}, \tag{84}$$

$$\Pi_{k+1} = F2_k^T \left(\Pi_k - \frac{h}{2} M_k \right) - \frac{h}{2} M_{k+1}, \tag{85}$$

$$\begin{aligned} \Pi2_{k+1} = {} & F2_k^T \left(\Pi2_k + \frac{h}{2} X_k \times \frac{\partial U}{\partial X_k} + \frac{h}{2} M_k \right) \\ & + \frac{h}{2} X_{k+1} \times \frac{\partial U}{\partial X_{k+1}} + \frac{h}{2} M_{k+1}, \end{aligned} \tag{86}$$

$$R_{k+1} = F2_k^T F_k R_k, \tag{87}$$

$$hS\left(\Pi_k - \frac{h}{2} M_k \right) = F_k J_{dR_k} - J_{dR_k} F_k^T, \tag{88}$$

$$hS\left(\Pi2_k + \frac{h}{2} X_k \times \frac{\partial U}{\partial X_k} + \frac{h}{2} M_k \right) = F2_k J_{d_2} - J_{d_2} F2_k^T. \tag{89}$$

It is natural to express the equations of motion for the second body in the inertial frame for reconstruction:

$$x2_{k+1} = x2_k + h\frac{\gamma2_k}{m_2} + \frac{h^2}{2m_2} R_k \frac{\partial U_k}{\partial X_k}, \tag{90}$$

$$\gamma2_{k+1} = \gamma2_k + \frac{h}{2} R_k \frac{\partial U_k}{\partial X_k} + \frac{h}{2} R_{k+1} \frac{\partial U_{k+1}}{\partial X_{k+1}}, \tag{91}$$

$$R2_{k+1} = R2_k F2_k. \tag{92}$$

Given $(R_0, X_0, \Pi_0, \Gamma_0, \Pi2_0)$, we can determine F_0 and $F2_0$ by solving the implicit equations (88) and (89). Then, X_1 and R_1 are found from (83) and (87), respectively. After that, we can compute Γ_1, Π_1, and $\Pi2_1$ from (84), (85) and (86). This yields a discrete Hamiltonian map $(R_0, X_0, \Pi_0, \Gamma_0, \Pi2_0) \mapsto (R_1, X_1, \Pi_1, \Gamma_1, \Pi2_1)$, and this process can be repeated. The discrete evolution of x_{2_k}, γ_{2_k} and R_{2_k} can be obtained as a post-processing step by using the reconstruction equations (90), (91) and (92), respectively.

3.3 Numerical considerations

Properties of the variational integrators: Since the LGVI is obtained by discretizing Hamilton's principle, it is symplectic and preserves the structure of the configuration space, SE(3), as well as the relevant geometric features of the full two rigid body problem, and the conserved first integrals of total linear and angular momenta and total energy. The total energy oscillates around its initial value with small bounds on a comparatively short timescale, but there is no tendency for the mean of the oscillation in the total energy to drift (increase or decrease) from the initial value for exponentially long time.

The LGVI preserves the group structure. By using the computational approach described in Sect. 3.4, the matrices F_{i_k} representing the change in relative attitude are guaranteed to be rotation matrices. The group operation of the Lie group SO(3) is matrix multiplication. Hence rotation matrices R_{i_k} are updated by the group operation, so that they evolve on SO(3) automatically without constraints or reprojection. Therefore, the orthogonal structure of the rotation matrices is preserved, and the attitude of each rigid body is determined accurately and globally without the need to use local charts (parameterizations) such as Euler angles or quaternions. These exact geometric properties of the discrete flow not only generate improved qualitative behavior, but also allow for accurate long-time simulation.

This geometrically exact numerical integration method yields a highly efficient and accurate computational algorithm for the full rigid body problem. For arbitrary shaped rigid bodies such as binary asteroids, there is a large burden in computing the mutual gravitational forces and moments, so the number of force and moment evaluations should be minimized. We have seen that the LGVI requires only one such evaluation per integration step, the minimum number of evaluations consistent with the presented LGVI having second order accuracy (because it is a self-adjoint method). Within the LGVI, implicit equations must be solved at each time step to determine the matrix-multiplication updates for rotation matrices. However the LGVI is only weakly implicit in the sense that the iteration for each implicit equation is independent of the much more costly gravitational force and moment computation. The computational load to solve each implicit equation is negligible; only two or three iterations are typically required. We make this more explicit in Sect. 3.4 by expressing F_{i_k} as the exponential function of an element of the Lie algebra $\mathfrak{so}(3)$. Altogether, the entire method could be considered *almost explicit*.

The LGVI is a fixed step size integrator, but all of the properties above are independent of the step size. Consequently, we can achieve the same level of accuracy while choosing a larger step size as compared to other numerical integrators of the same order.

All of these features are revealed by numerical simulations in Sect. 4 and in the work by Fahnestock et al. (2006). In Sect. 4, the LGVI is compared with other second order geometric integrators: a symplectic Runge-Kutta method and a Lie group method. In Fahnestock et al. (2006), the LGVI is directly compared with the 7(8)th order Runge-Kutta-Fehlberg method (RK78) for two octahedral rigid bodies. It is shown that the LGVI requires 8 times less computational load than RK78 for similar error measures, and the accuracy of the LGVI is maintained for exponentially long time. The trajectories computed using RK78 are unreliable for the long time simulation of the full two rigid body dynamics.

Higher-order methods: While the numerical methods we present in this paper are second order, it is possible to apply symmetric composition methods, introduced by Yoshida (1990), to construct higher-order versions of the Lie group variational integrators introduced here. Given a basic numerical method represented by the flow map Φ_h, the composition method is obtained by applying the basic method using different step sizes,

$$\Psi_h = \Phi_{\lambda_s h} \circ \ldots \circ \Phi_{\lambda_1 h},$$

where $\lambda_1, \lambda_2, \cdots, \lambda_s \in \mathbb{R}$. In particular, the Yoshida symmetric composition method for composing a symmetric method of order 2 into a symmetric method of order 4 is obtained when $s = 3$, and

$$\lambda_1 = \lambda_3 = \frac{1}{2 - 2^{1/3}}, \qquad \lambda_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}.$$

Alternatively, by adopting the formalism of higher-order Lie group variational integrators introduced by Leok (2004) in conjunction with the Rodrigues formula, one can directly construct higher-order generalizations of the Lie group methods presented here.

Reduction of orthogonality loss due to roundoff error: In Lie group variational integrators, the numerical solution is made to automatically remain on the rotation group by requiring that the numerical solution is updated by matrix multiplication with the exponential of a skew-symmetric matrix.

Since the exponential of a skew-symmetric matrix is orthogonal to machine precision, the numerical solution will only deviate from orthogonality due to the accumulation of roundoff error in the matrix multiplication, and this orthogonality loss grows linearly with the number of timesteps taken. The phenomena can be observed in the numerical simulations described in Fig. 3(c) of Sect. 4, wherein the orthogonality error for the Lie group method and the Lie group variational integrator increases as the step size decreases, due to the roundoff error accumulation as the number of matrix multiplications increase.

One possible method of addressing this issue is to use the Baker-Campbell-Hausdorff (BCH) formula to track the updates as skew-symmetric matrices (the Lie algebra). This allows us to find a matrix $C(t)$, such that,

$$\exp(tA)\exp(tB) = \exp C(t).$$

This matrix $C(t)$ satisfies the following differential equation,

$$\dot{C} = A + B + \frac{1}{2}[A - B, C] + \sum_{k \geq 2} \frac{B_k}{k!} \operatorname{ad}_C^k (A + B),$$

with initial value $C(0) = 0$, where B_k denotes the Bernoulli numbers and $\operatorname{ad}_C A = [C, A] = CA - AC$.

The problem with this approach is that the matrix $C(t)$ is not readily computable for arbitrary A and B, and in practice, the series is truncated, and the differential equation is solved numerically.

An error is introduced in truncating the series, and numerical errors are introduced in numerically integrating the differential equations. Consequently, while the BCH formula could be used solely at the reconstruction stage to ensure that the numerical attitude always remains in the rotation group to machine precision, the truncation error would destroy the symplecticity and momentum preserving properties of the numerical scheme.

However, by combining the BCH formula with the Rodrigues formula in constructing the discrete variational principle, it might be possible to construct a Lie group variational integrator that tracks the reconstructed trajectory on the rotation group at the level of a curve in the Lie algebra, while retaining its structure-preservation properties.

3.4 Computational approach

The structure of the discrete equations of motion given in (57), (62), (78), (79), (88), and (89) suggests a specific computational approach. For a given $g \in \mathbb{R}^3$, we have to solve the following Lyapunov-like equation to find $F \in \mathrm{SO}(3)$ at each integration step.

$$FJ_d - J_d F^T = S(g). \tag{93}$$

This equation is linear in F, but it is implicit due to the nonlinear constraint $F^T F = I_{3\times 3}$. We now introduce two iterative approaches to solve (93) numerically.

Exponential map: An element of a Lie group can be expressed as the exponential of an element of its Lie algebra, so $F \in \mathrm{SO}(3)$ can be expressed as an exponential of $S(f) \in \mathfrak{so}(3)$ for some vector $f \in \mathbb{R}^3$. The exponential can be written in closed form, using Rodrigues' formula,

$$F = \exp S(f) = I_{3\times 3} + \frac{\sin\|f\|}{\|f\|} S(f) + \frac{1-\cos\|f\|}{\|f\|^2} S(f)^2. \tag{94}$$

Substituting (94) into (93), we obtain

$$S(g) = \frac{\sin\|f\|}{\|f\|} S(Jf) + \frac{1-\cos\|f\|}{\|f\|^2} S(f \times Jf).$$

Thus, (93) is converted into the equivalent vector equation $g = G(f)$, where $G : \mathbb{R}^3 \mapsto \mathbb{R}^3$ is given by

$$G(f) = \frac{\sin\|f\|}{\|f\|} Jf + \frac{1-\cos\|f\|}{\|f\|^2} f \times Jf. \tag{95}$$

We use the Newton method to solve $g = G(f)$, which gives the iteration

$$f_{i+1} = f_i + \nabla G(f_i)^{-1} \left(g - G(f_i)\right). \tag{96}$$

We iterate until $\|g - G(f_i)\| < \epsilon$ for a small tolerance $\epsilon > 0$. The Jacobian $\nabla G(f)$ in (96) can be expressed as

$$\begin{aligned}\nabla G(f) = \; & \frac{\cos\|f\|\,\|f\| - \sin\|f\|}{\|f\|^3} Jff^T + \frac{\sin\|f\|}{\|f\|} J \\ & + \frac{\sin\|f\|\,\|f\| - 2(1-\cos\|f\|)}{\|f\|^4} (f \times Jf) f^T \\ & + \frac{1-\cos\|f\|}{\|f\|^2} \left\{-S(Jf) + S(f)J\right\}.\end{aligned}$$

Cayley transformation: Similarly, given $f_c \in \mathbb{R}^3$, the Cayley transformation is a local diffeomorphism that maps $S(f_c) \in \mathfrak{so}(3)$ to $F \in \mathrm{SO}(3)$, where

$$F = \operatorname{cay} S(f_c) = (I_{3\times 3} + S(f_c))(I_{3\times 3} - S(f_c))^{-1}. \tag{97}$$

Substituting (97) into (93), we obtain a vector equation $G_c(f_c) = 0$ equivalent to (93)

$$G_c(f_c) = g + g \times f_c + (g^T f_c) f_c - 2J f_c = 0, \tag{98}$$

and its Jacobian $\nabla G_c(f_c)$ is written as

$$\nabla G_c(f_c) = S(g) + (g^T f_c) I_{3\times 3} + f_c g^T - 2J.$$

Then, (98) is solved by using Newton's iteration (96), and the rotation matrix is obtained by the Cayley transformation.

For both methods, numerical experiments show that 2 or 3 iterations are sufficient to achieve a tolerance of $\epsilon = 10^{-15}$. Numerical iteration with the Cayley transformation is a little faster due to the simpler expressions. It should be noted that since $F = \exp S(f)$ or $F = \operatorname{cay} S(f_c)$, it is automatically a rotation matrix, even when the equation $g = G(f)$ is not satisfied to machine precision.

These computational approaches are distinguished from solving the implicit equation (93) with 9 variables and 6 constraints. Due to their numerical efficiency, the Lie group variational integrator can be considered an almost explicit computational method as demonstrated in the next section.

4 Numerical simulations

We simulate the dynamics of two simple dumbbell bodies acting under their mutual gravity. Each dumbbell model consists of two equal rigid spheres and a rigid massless connecting rod. This dumbbell rigid body model has a simple closed form for the mutual gravitational potential given by

$$U(X,R) = -\sum_{p,q=1}^{2} \frac{G m_1 m_2/4}{\left\| X + \rho_{2_p} + R\rho_{1_q} \right\|},$$

where G is the universal gravitational constant, $m_i \in \mathbb{R}$ is the total mass of the ith dumbbell, and $\rho_{i_p} \in \mathbb{R}^3$ is a vector from the origin of the body-fixed frame to the pth sphere of the ith dumbbell in the ith body-fixed frame. The vectors $\rho_{i_1} = [l_i/2, 0, 0]^T$, $\rho_{i_2} = -\rho_{i_1}$, where l_i is the length between the two spheres. Mass, length and time dimensions are normalized.

The mass and length of the second dumbbell are twice that of the first dumbbell. The other simulation parameters are chosen such that the total linear momentum in the inertial frame is zero and the relative motion between two bodies are near-elliptic orbits. The trajectories of dumbbell bodies are shown in Fig. 2.

We compare the computational properties of the Lie group variational integrator (LGVI) with other second order numerical integration methods; an explicit Runge-Kutta method (RK), a symplectic Runge-Kutta method (SRK), and a Lie group method (LGM). One of the distinct features of the LGVI is that it preserves both the symplectic property and the Lie group structure of the full rigid body dynamics. A comparison can be made between the LGVI and other integration methods that

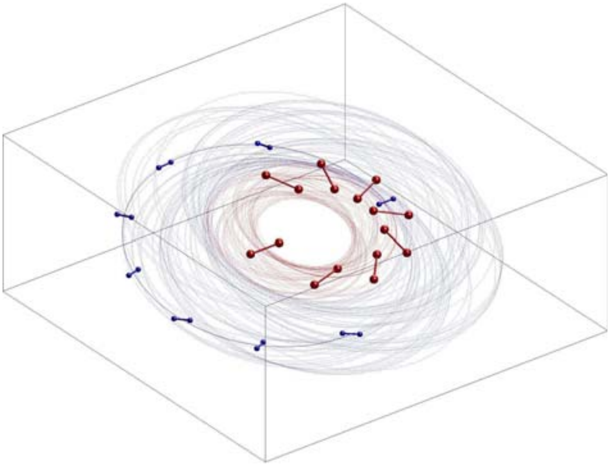
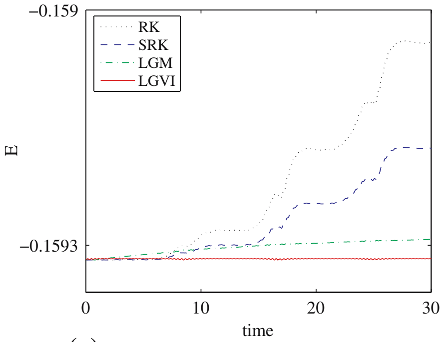


Fig. 2 Trajectories of two dumbbell bodies in the inertial frame (The initial orbit is shown with solid lines and snapshots of dumbbell body maneuver. A simple animation is available at http://www.umich.edu/ tylee.)

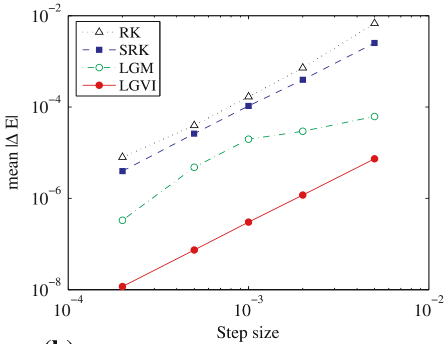
preserve either none or one of these properties: an integrator that does not preserve any of these properties (RK), a symplectic integrator that does not preserve the Lie group structure (SRK), and a Lie group integrator that does not preserve symplecticity (LGM). These methods are implemented by an explicit mid-point rule, an implicit mid-point rule, and the Crouch-Grossman method presented in (Hairer et al. 2006) for the continuous equations of motion (40)–(48), respectively. For the LGVI, the discrete equations of motion given by (83) through (92) are used. All of these integrators are second order accurate. A comparison with a higher-order integrator can be found in (Fahnestock et al. 2006).

Fig. 3(a) shows the computed total energy response over 30 seconds with an integration step size $h = 0.002$ sec. For the LGVI, the total energy is nearly constant, and there is no tendency to drift, while the other integrators fail to preserve the total energy. This can be observed in Fig. 3(b), where the mean total energy deviations are shown for varying integration step sizes. It is seen that the total energy errors of the SRK method is close to the RK method, but the total energy error of the LGVI is smaller by several orders. Fig. 3(c) shows the mean orthogonality errors. The LGVI and the LGM conserve the orthogonal structure at an error level of 10^{-10}, while the RK and the SRK do not.

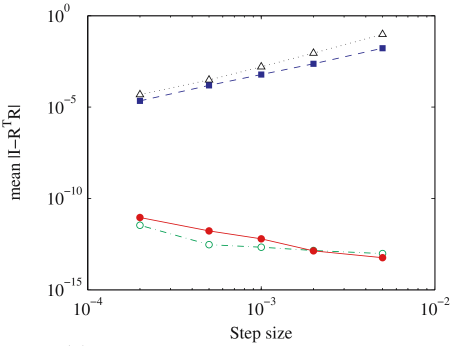
These computational comparisons suggest that for numerical integration of Hamiltonian systems evolving on a Lie group, such as full body problems, it is critical to preserve both the symplectic property and the Lie group structure. For the RK and the SRK, the orthogonality error in the rotation matrix corrupts the attitude of the rigid bodies. The accumulation of this attitude degradation causes significant errors in the computation of the gravitational forces and moments dependent upon the position and the attitude, which affect the accuracy of the entire numerical simulation. The LGM conserves the orthogonal structure of rotation matrices numerically, but it does not respect the characteristics of the Hamiltonian dynamics properly as a non-symplectic integrator; this causes a drift of the computed total energy. The LGVI is a geometrically exact integration method in the sense that it preserves all of the



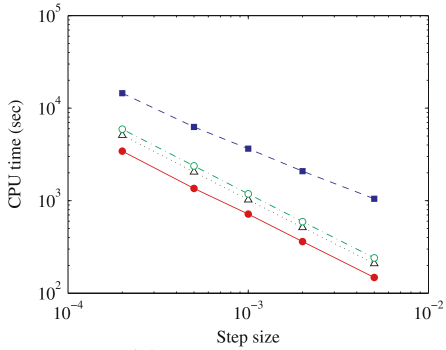
(a) Computed total energy for 30 seconds



(b) Mean total energy error $|E - E_0|$ vs. step size



(c) Mean orthogonality error $\|I - R^T R\|$ vs. step size



(d) CPU time vs. step size

Fig. 3 Computational properties of explicit Runge-Kutta (RK), symplectic Runge-Kutta (SRK), Lie group method (LGM), and Lie group variational integrator (LGVI)

features of the full rigid body dynamics concurrently. This verifies the superiority of the LGVI in terms of computational accuracy. The performance advantages of the LGVI becomes even more dramatic as the simulation time is increased.

Computational efficiency is compared in Fig. 3(d), where CPU times of all methods are shown for varying step sizes. The SRK has the largest CPU time requiring solution of an implicit equation in 36 variables at each integration step. The RK and the LGM require similar CPU times since both are explicit. It is interesting to see that the implicit LGVI actually requires less CPU time than the explicit methods RK and LGM. This follows from the fact that the second order explicit methods RK and LGM require two evaluations of (40)–(48), including the expensive force and moment computations at each step. The LGVI requires only one evaluation at each step in addition to the solution the implicit equation. The computational approach described in Sect. Fig. 3 is efficient for solving the implicit equation (93) and hence it takes less time than the evaluation of (40)–(48). The difference is further increased as the rigid body model becomes more complicated since it involves a larger computation burden in computing the gravitational forces and moments. Based on these properties, we claim that the LGVI is *almost explicit*. This comparison demonstrates the higher computational efficiency of the LGVI.

In summary, comparing both Fig. Fig. 3(b) and (d), we see that the LGVI requires 16 times less CPU time than the LGM, 35 times less CPU time than the RK, and 98 times less CPU time than the SRK for similar total energy error in this computational example for the full body problem.

5 Conclusions

Eight different forms of the equations of motion for the full body problem are derived. The continuous equations of motion and variational integrators are derived both in inertial coordinates and in relative coordinates, and each set of equations of motion is expressed in both Lagrangian and Hamiltonian form.

It is shown that both of the continuous equations and the discrete equations of motion for the full body problem can be derived systematically, using proper variations of Lie group elements, according to Hamilton's principle. The proposed Lie group variational integrators are geometrically exact; they preserve the momenta and symplectic form of the continuous dynamics, exhibit good energy properties, and they also conserve the geometry of the configuration space. They provide a numerically efficient computational approach especially for the full body problems in the sense that they require only one evaluation of mutual gravity forces and moments per step. The exact geometric properties of the discrete flow not only yields improved qualitative behavior, but also allow for accurate long-time simulation. The numerical example verifies the substantial superiority of the Lie group variational integrator compared with other geometric integrators in terms of computational accuracy and efficiency.

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