Research Inventy: International Journal of Engineering And Science
Vol.10, Issue 10 (October 2020), PP 72-76
Issn (e): 2278-4721, Issn (p):2319-6483, www.researchinventy.com

The stability of exponential variational integrators as key role tool in studying multibody holonomic systems

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Abstract: *The role of stability of high order exponential variational integrators (EVIs) when they are applied to mechanical systems with holonomic constraints, is extensively examined and discussed. This class of geometric type integration schemes are determined through a discretization of the variational Hamilton's principle and the definition of a characteristic discrete Lagrangian. The formulation of exponential interpolation functions is tested on the discrete Euler-Lagrangian equations in the presence of constraints. The resulting schemes are then applied on dynamical multibody systems with holonomic constraints, choosing the double pendulum as a concrete example. The long-time behavior of the EVIs, which reflects their property of stability was found to be very good compared to that of other traditional methods.*
Keywords: *Variational integrators, High order geometric integrators, Discrete variational mechanics, Multibody system, Systems with Constraints*

Date of Submission: 09-10-2020 Date of Acceptance: 24-10-2020

I. INTRODUCTION

During the last decades, great emphasis has been given by researches, to the time and space discretization in treating numerically the Lagrange and Hamilton methods and solve the differential equations governing the mechanical system in question. To this aim, obviously one needs first to define the discrete analogue of the continuous methods, like discrete variational calculus, discrete Lagrangian and Hamiltonian functions, the discrete Hamilton principle etc. (Marsden and West, 2010; Heirer et al., 2003; Kosmas and Leyendecker, 2016; Kosmas and Leyendecker, 2019; Kosmas and Leyendecker, 2016).

In recent years, for the solution of mechanical systems numerical methods that preserve the underlying geometric structure of the system are widely used. As a special case, the class of the variational integrators have been proven to be symplectic and momentum preserving (Engquist et al., 2009; Kane et al., 2001).

When solving conservative problems these methods are derived by mimicking the continuous Hamilton's principle, while for dissipative and/or controlled mechanical systems the Lagrange-d'Alembert principle is preferable. Both approaches lead to discrete versions of the known principles (Leyendecker et al., 2004; Junge et al., 2005, Schmidt et al., 2009). In order to improve the accuracy of the standard variational integrators, high order schemes can be derived via the approximation of the action on a finite-dimensional function space and use of numerical quadrature formulas (Stern and Grinspun, 2009).

In our previus work we have proposed exponential variational integrators derived by using a discrete Lagrangian defined as a weighted sum over continuous Lagrangians evaluated inbetween number of intermediate points (Kosmas and Leyendecker, 2016; Kosmas and Leyendecker, 2019; Kosmas and Leyendecker, 2016). The accuracy of these EVIs (Kosmas and Vlachos, 2012; Kosmas and Papadopoulos, 2014; Kosmas and Leyendecker, 2012; Kosmas and Leyendecker, 2014; Kosmas, 2011), especially for long term integration, is very good as has been shown from the comparison of their results with those of several similar variational integrators (Hochbruck et al., 1998; Kosmas, 2020; Kosmas et al., 2020).

In the present article, we make an effort to extend such numerical schemes so as to become applicable to conservative mechanical systems. Initially we focus on cases where holonomic constraints are present. To this purpose, we first define the continuous and the discrete versions of the Euler-Lagrangian equations for such systems (Section 2), and then we use them for the proposed high order schemes described (Section 3). Finally, we test the derived schemes on the numerical solution of the double pendulum system and compare their efficiency with that of some standard methods.

II. REVIEW OF MULTIBOBY SYSTEM DYNAMICS WITH HOLONOMIC CONSTRAINTS

We here turn our interest on multibody system dynamics with holonomic constraints. From those we will use Hamilton's principle as expressed via the variation of the action S

$$\delta S = \delta \int_{t_0}^{t} \left(L(q,\dot{q},t) - \lambda^T \varphi(q,t)\right)dt = 0 \qquad (1)$$

In the latter equation, the q and $\dot{q}$ are the generalized displacements and velocities respectively, while L denotes the Lagrangian of the system. Additionally φ is the expression of the constraints, which we will consider as $\varphi(q,t) = 0$ and is then used in (1) by adding a Lagrange multiplier λ. The described variational method leads to the Euler-Lagrange equations which can be written as

$$\frac{d}{dt}\left(\frac{\partial L(q,\dot{q},t)}{\partial \dot{q}}\right) - \frac{\partial L(q,\dot{q},t)}{\partial q} + \varphi^T(q,t)\lambda = 0$$
$$\varphi(q,t) = 0 \qquad (2)$$

and then solved using numerical methods, see (Leyendecker et al., 2008).

The proposed geometric scheme mimics the steps of the continuous formalism. Thus we first make use of the time step h that divides the time integral $[t_0, t]$ into N subintervals,

$$t_i = ih, \quad \mathrm{i} = 0,1,2,\ldots,\mathrm{N}, \quad N \in \mathbb{N}. \qquad (3)$$

We then define

$$q_i = q(t_i) \qquad \text{and} \qquad \dot{q}_i = \dot{q}(t_i) \qquad (4)$$

the discrete configurations and velocities respectively and the discrete versions of the Lagrange multipliers using

$$\lambda_i = \lambda(t_i). \qquad (5)$$

For a smooth and finite dimensional configuration manifold Q we can then define the discrete Lagrangian

$$L_d : Q \times Q \longrightarrow \mathbb{R}, \qquad (6)$$

as an approximation of a continuous action, thus

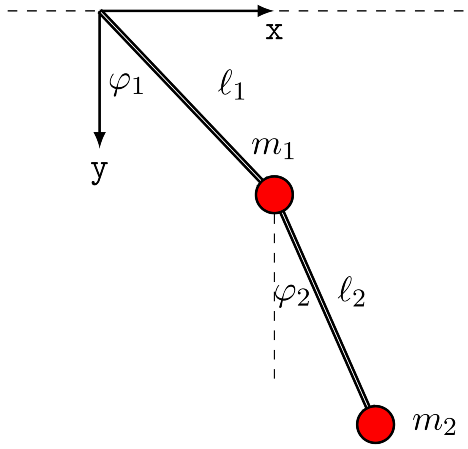
$$L_d(q_k, q_{k+1}, h) \doteq \int_{t_k}^{t_{k+1}} L(q,\dot{q})dt. \qquad (7)$$

Using the discrete variational principle, the solutions of the discrete system are determined from L_d by extremizing the discrete action sum, keeping the endpoints q_0 and q_N fixed. The resulting discrete Euler-Lagrange equations are then

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) - h\varphi_q^T(q_k)\lambda_k = 0$$
$$\varphi(q_{k+1}) = 0, \qquad (8)$$

where $k = 1,\ldots,N-1$ and D_i stands for the derivative with respect to the i-argument of L_d, see (Leyendecker et al., 2008) and (Kosmas, 2019).

Figure1. Double pendulum system.



III. HIGH ORDER EXPONENTIAL VARIATIONAL INTEGRATORS

In order to extend the variational integrators to arbitrary and thus high orders an approximation of the action integral along the curve segment between q_k and q_{k+1} must be considered. That can happen by Introducing intermediate points which are then used for the expressions for the configurations configurations q_k^j and velocities $\dot{q}_k^j$, $j = 0,\ldots,S-1$, $\mathrm{S} \in \mathbb{N}$, at time $t_k^j \in [t_k^j, t_{k+1}^j]$. In addition we define t_k^j as

$$t_k^j = t_k + C_k^j h_k, \qquad (9)$$

using $C_k^j \in [0,1]$ such that

$$C_k^0 = 0, C_k^1 = 1, \qquad (10)$$

which also defines a time step $h \in \mathbb{R}$.

Exponential variational integrators of high order arew then defined using

$$q_k^j = g_1(t_k^j)q_k + g_2(t_k^j)q_{k+1}, \quad (11)$$

and

$$\dot{q}_k^j = \dot{g}_1(t_k^j)q_k + \dot{g}_2(t_k^j)q_{k+1}\,. \quad (12)$$

for (Kosmas and Leyendecker, 2019; Kosmas, 2020)

$$g_1(t_k^j) = \sin\left(u - \frac{t_k^j - t_k}{h_k}u\right)\sin^{-1}(u), \quad (13)$$

and

$$g_2(t_k^j) = \sin\left(\frac{t_k^j - t_k}{h_k}u\right)\sin^{-1}(u). \quad (14)$$

For the sake of continuity, the conditions

$$g_1(t_{k+1}) = g_2(t_k) = 0 \quad \text{and} \quad g_1(t_k) = g_2(t_{k+1}) = 1 \quad (15)$$

are required to be fulfilled (Kosmas and Leyendecker, 2012; Kosmas and Vlachos, 2012; Kosmas and Leyendecker, 2015). We can then define discrete Lagrangian L_d by a weighted sum of the form (Kosmas and Leyendecker, 2019; Kosmas 2020)

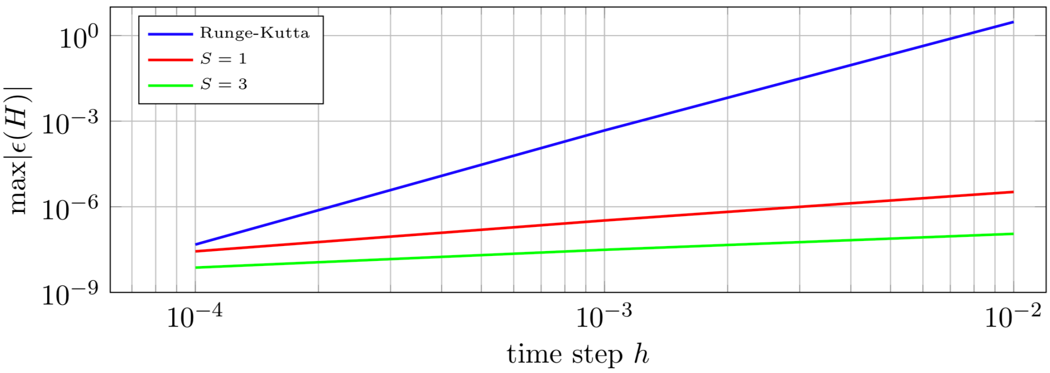
$$L_d(q_k, q_{k+1}, h_k) = \sum_{j=0}^{S-1} h_k w^j L\left(q(t_k^j), \dot{q}(t_k^j)\right), \quad (16)$$

where, as can be readily proved, it holds (Kosmas and Leyendecker, 2012; Kosmas and Leyendecker, 2016; Kosmas and Leyendecker, 2019)

$$\sum_{j=0}^{S-1} w^j (C_k^j)^m = \frac{1}{m+1}, \quad (17)$$

with m=0,1,...,S-1 and m=0,1,...,N-1.

Figure2. Maximum of total energy errors.



IV. NUMERICAL RESULTS

As a numerical test we consider the planar double pendulum system of (Hairer et al., 2003), see Figure 1, and denoting the masses and lengths by m_1, m_2 and l_1, l_2 respectively (all masses and lengths are considered to be ones). Writing the configuration positions as

$$q = [x_1 \;\; y_1 \;\; x_2 \;\; y_2]^T, \quad (18)$$

the kinetic energy of the system can be written as

$$T(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q}, \quad (19)$$

for the mass matrix

$$M = \begin{bmatrix} m_1 & 0 & 0 & 0 \\ 0 & m_2 & 0 & 0 \\ 0 & 0 & m_3 & 0 \\ 0 & 0 & 0 & m_4 \end{bmatrix}. \quad (20)$$

The potential, using the gravitational constant g, is

$$V(q) = m_1 g y_1 + m_2 g y_2. \quad (21)$$

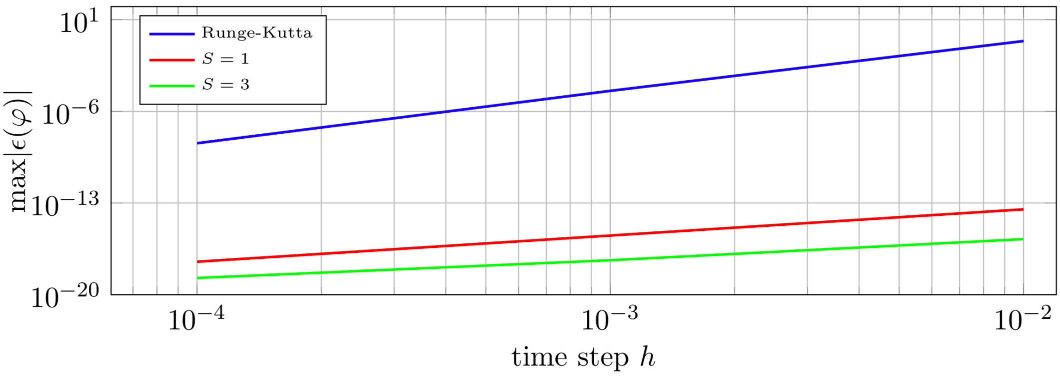
For that equation for the constraints of (2) can be written as

$$\varphi(q) = \begin{bmatrix} x_1^2 + y_1^2 - l_1^2 \\ (x_2 - x_1)^2 + (y_2 - y_1)^2 - l_2^2 \end{bmatrix} = 0. \quad (22)$$

We can now define the discrete Lagrangian of (16) which is then used to the discrete Euler-Lagrange equations of (5) in order to obtain the solution of the physical problem.

To test the proposed method we consider two different number of intermediate points at each time segments $[t_k, t_{k+1}]$ of the discrete Lagrangian (16), i.e. $S = 1$ and $S = 3$. As described in Section 3 the first corresponds to one intermediate point while the second to three. For those methods in Figure 2 we plot the maximum error of the total energy H of the system, $max|\varepsilon(H)|$, after 100 steps and compare them with the ones obtained using a standard Runge-Kutta method, see (Hairer et al., 2003). For the time steps chosen here, thus $h = 10^{-1}, h = 10^{-2}$ and $h = 10^{-3}$ the energy errors obtained from the proposed schemes converge to much smaller values. Same results are obtained in Figure 3, where the maximum error of the constrained equation, i.e. $max|\varepsilon(\varphi)|$ is presented.

Figure3. Maximum of errors for constraints.



V. CONCLUSION AND FUTURE WORK

We examined the key role of the stability of exponential variational integrators when they are properly formulated for the numerical solution of multibody dynamical system with constraints. To do so we first defined a discrete Lagrangian that describes the physical problem, which is then combined with a discrete version of the constraints on a standard setting of the discrete Euler-Lagrangian equations with holonomic constraints. Finally, for the solution of the double pendulum system results obtained with methods of different numerical order, show that the proposed schemes preserve their good behavior when compared to other traditional methods.

Conflict of interest

There is no conflict to disclose.

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