Variational Integrators as General Linear Methods

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Abstract

In this paper we write variational integrators for degenerate Lagrangian systems as general linear methods which turn out to be G-symplectic in nature. Since variational integrators for degenerate Lagrangian systems suffer from parasitic instabilities, we use the G-symplectic general linear method formulation to calculate their parasitic growth parameters, thus enabling us to devise strategies to control numerical instabilities while preserving the underling physical laws of the system. Variational integrators based on trapezoidal and mid-point quadrature rules are considered for degenerate Lagrangian systems resulting in two different classes of general linear methods. We then apply the standard projection technique to project the numerical solution on whatever manifold the exact solution lies on, resulting in energy preservation for long time. The numerical results verify our claims.

Keywords: Variational integrator, degenerate Lagrangian, general linear method, parasitism, projection technique

1. Introduction

Variational integrators for non-degenerate Lagrangian systems result in symplectic one-step methods [15]. In the following we show that variational integrators for degenerate Lagrangian systems result in G-symplectic general linear methods.

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Let us consider a degenerate Lagrangian system whose Lagrangian is linear in velocities and has the form,

$$L(q,\dot{q}) = \langle \alpha(q), \dot{q} \rangle - H(q), \qquad \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} = 0, \qquad L : TQ \to R, \tag{1}$$

where α can be a nonlinear function of position $q(t) \in Q$, and $H(q)$ is the Hamiltonian of the system. Hamilton's principle of least action can be applied on (1) which leads to the Euler-Lagrange equations given as,

$$\frac{\partial L}{\partial q}(q,\dot{q}) - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}(q,\dot{q}) = 0. \tag{2}$$

In the variational integrator methodology, first the action integral of the degenerate Lagrangian system (1) is discretised. Then the application of the discrete Hamilton's principle of stationary action results in the discrete Euler Lagrange equations, which produce the required variational integrators for degenerate Lagrangian systems. These integrators are multistep numerical methods having parasitic instabilities.

The nature of the particular multistep method depends upon the choice of quadrature rule to approximate the action integral. If we choose trapezoidal rule, we obtain standard linear multistep method, whereas the choice of midpoint rule results in a two step Runge–Kutta method, both of which can be written as G-symplectic general linear methods [12, 13, 14, 15, 16]. We then apply the projection technique [1, 9, 10] to control the effects of parasitism [4, 6]. This approach has the advantage that the resulting methods are applicable to all degenerate Lagrangians of the form (1).

2. Variational Integrators for Degenerate Lagrangian Systems

Let us consider the action integral which is given as,

$$A[q(t)] = \int L(q(t), \dot{q}(t))dt, \tag{3}$$

and discretise it to obtain

$$A_d[q_d] = \sum_{m=0}^{N-1} L_d(q_m, q_{m+1}),$$

with the discrete Lagrangian L_d providing some approximation of the continuous Lagrangian L,

$$L_d(q_m, q_{m+1}) \approx \int_{t_m}^{t_{m+1}} L(q(t), \dot{q}(t))dt, \tag{4}$$

where $L_d : Q \times Q \to R$. Here, we divide the time interval into an equidistant monotonic sequence $\{t_m\}_{m=0}^N$ and approximate the solution at each point in time as $q_m \approx q(t_m)$ leading to the discrete trajectory $\{q_m\}_{m=0}^N$ joined by a discrete curve and then sum the discrete Lagrangian $L_d(q_m, q_{m+1})$ on each adjacent pair. The velocities are approximated using finite differences as,

$$\dot{q} \approx \frac{q_{m+1} - q_m}{h},$$

where $h = t_{m+1} - t_m \; \forall m$ is the time step size. We approximate the the integral in (4) using quadrature rules such as the trapezoidal rule to obtain the discrete Lagrangian L_d^{tr} given as,

$$L_d^{tr}(q_m, q_{m+1}) = \frac{h}{2}[L(q_m, \frac{q_{m+1} - q_m}{h}) + L(q_{m+1}, \frac{q_{m+1} - q_m}{h})], \tag{5}$$

or the midpoint rule to obtain to obtain the discrete Lagrangian L_d^{mp} given as,

$$L_d^{mp}(q_m, q_{m+1}) = h[L(\frac{q_m + q_{m+1}}{2}, \frac{q_{m+1} - q_m}{h})], \tag{6}$$

The discrete trajectories $\{q_m\}_{m=0}^N$ satisfy a discrete version of Hamilton's principle of stationary action which require $\delta A_d[q_d] = 0$. The variation is given as,

$$\begin{aligned}
\delta A_d[q_d] &= \delta \sum_{m=0}^{N-1} L_d(q_m, q_{m+1}), \\
&= \sum_{m=0}^{N-1} [D_1 L_d(q_m, q_{m+1}) \cdot \delta q_m + D_2 L_d(q_m, q_{m+1}) \cdot \delta q_{m+1}],
\end{aligned}$$

Here an integration by parts is used, and D_1 and D_2 are the derivatives with respect to the first and the second arguments respectively. Applying integration by parts and using that the variations at the endpoints are fixed so $\delta q_0 = \delta q_N = 0$, we obtain,

$$\delta A_d[q_d] = \sum_{m=1}^{N-1} [D_1 L_d(q_m, q_{m+1}).\delta q_m + D_2 L_d(q_{m-1}, q_m)].\delta q_m.$$

By invoking the Hamilton's principle of stationary action which requires $\delta A_d = 0$ for all δq_d, we obtain discrete Euler-Lagrange equations,

$$D_1 L_d(q_m, q_{m+1}) + D_2 L_d(q_{m-1}, q_m) = 0. \tag{7}$$

2.1. Trapezoidal Rule

For the special case of degenerate Lagrangian system (1), we have for trapezoidal rule,

$$L_d^{tr}(q_m, q_{m+1}) = \frac{h}{2}[\alpha(q_m) \cdot \frac{q_{m+1} - q_m}{h} - H(q_m) + \alpha(q_{m+1}) \cdot \frac{q_{m+1} - q_m}{h} - H(q_{m+1})],$$

with the differentiation operators given as,

$$D_1 L_d^{tr}(q_m, q_{m+1}) = \frac{h}{2}[\nabla\alpha(q_m) \cdot \frac{q_{m+1} - q_m}{h} - \frac{\alpha(q_m)}{h} - \frac{\alpha(q_{m+1})}{h} - \nabla H(q_m)],$$
$$D_2 L_d^{tr}(q_{m-1}, q_m) = \frac{h}{2}[\nabla\alpha(q_m).\frac{q_m - q_{m-1}}{h} + \frac{\alpha(q_m)}{h} + \frac{\alpha(q_{m-1})}{h} - \nabla H(q_m)].$$

The discrete Euler-Lagrange equation (7) results in the following variational integrator using the trapezoidal rule,

$$\nabla\alpha(q_m).(q_{m+1} - q_{m-1}) = \alpha(q_{m+1}) - \alpha(q_{m-1}) + 2h\nabla H(q_m). \tag{8}$$

2.2. Midpoint Rule

The use of midpoint quadrature rule results in,

$$L_d^{mp}(q_m, q_{m+1}) = h[\alpha(\frac{q_m + q_{m+1}}{2}).\frac{q_{m+1} - q_m}{h} - H(\frac{q_m + q_{m+1}}{2})],$$

with the differentiation operators given as,

$$D_1^{mp} L_d(q_m, q_{m+1}) = h[\frac{1}{2}\nabla\alpha(\frac{q_m + q_{m+1}}{2}).\frac{q_{m+1} - q_m}{h} - \frac{1}{h}\alpha(\frac{q_m + q_{m+1}}{2}) - \frac{1}{2}\nabla H(\frac{q_m + q_{m+1}}{2})],$$
$$D_2^{mp} L_d(q_{m-1}, q_m) = h[\frac{1}{2}\nabla\alpha(\frac{q_{m-1} + q_m}{2}).\frac{q_m - q_{m-1}}{h} + \frac{1}{h}\alpha(\frac{q_{m-1} + q_m}{2}) - \frac{1}{2}\nabla H(\frac{q_{m-1} + q_m}{2})].$$

The discrete Euler-Lagrange equation (7) results in the following variational integrator using the midpoint rule,

$$\frac{1}{2}\nabla\alpha(\frac{q_m + q_{m+1}}{2}) \cdot \frac{q_{m+1} - q_m}{h} + \frac{1}{2}\nabla\alpha(\frac{q_{m-1} + q_m}{2}).\frac{q_m - q_{m-1}}{h} =$$
$$\frac{1}{h}[\alpha(\frac{q_m + q_{m+1}}{2}) - \alpha(\frac{q_{m-1} + q_m}{2})] + \frac{1}{2}[\nabla H(\frac{q_m + q_{m+1}}{2}) + \nabla H(\frac{q_{m-1} + q_m}{2})]. \tag{9}$$

3. General Linear Methods

General linear methods are multi-value multi-derivative numerical methods for solving initial value problems [3, 11],

$$y' = f(y), \qquad y(0) = y_0, \tag{10}$$

where $f : \mathbb{R}^N \to \mathbb{R}^N$ and $x \in \mathbb{R}$. They have internal stages like Runge–Kutta methods and several input values like multi-step methods but they are more general in nature. An s-stage general linear method with r-component input vector has the general form,

$$\begin{aligned} Y &= h(A \otimes I) f(Y) + (U \otimes I) y^{[m-1]}, & Y \in (\mathbb{R}^N)^s \\ y^{[m]} &= h(B \otimes I) f(Y) + (V \otimes I) y^{[m-1]} & y \in (\mathbb{R}^N)^r \end{aligned} \tag{11}$$

The vector form of these quantities are,

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \qquad y^{[m]} = \begin{bmatrix} y_1{}^{[m]} \\ y_2{}^{[m]} \\ \vdots \\ y_r{}^{[m]} \end{bmatrix}.$$

The matrices (A, U, B, V) represents a particular general linear method where

$$M = \left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \tag{12}$$

is a $(s+r) \times (s+r)$ matrix tableau. We can omit the Kronecker products to write the general linear methods as,

$$\begin{aligned} Y &= hAf(Y) + Uy^{[m-1]}, \\ y^{[m]} &= hBf(Y) + Vy^{[m-1]}. \end{aligned}$$

A more convenient way of writing a general linear method is,

$$\left[\begin{array}{c} Y \\ \hline y^{[m]} \end{array}\right] = \left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \left[\begin{array}{c} hf(Y) \\ \hline y^{[m-1]} \end{array}\right]. \tag{13}$$

3.1. Runge-Kutta Methods as General Linear Methods

A Runge–Kutta method $[A,b,c]$ has s-stages and a single input with $r=1$ so that the matrices $U=\mathbf{1}\in(\mathbb{R}^N)^s$, $V=1$ and B is a single row vector $[b]$. Th general linear formulation of a Runge–Kutta method is,

$$\left[\begin{array}{c} Y \\ \hline y^{[m]} \end{array}\right] = \left[\begin{array}{c|c} A & \mathbf{1} \\ \hline b & 1 \end{array}\right] \left[\begin{array}{c} hf(Y) \\ \hline y^{[m-1]} \end{array}\right].$$

3.2. Linear Multistep Methods as General Linear Methods

A linear multistep method such as an Adams-Moulton method given as,

$$y_m = y_{m-1} + h(\beta_0 f(y_m) + \beta_1 f(y_{m-1}) + \beta_2 f(y_{m-2}) + \cdots + \beta_k f(y_{m-k})),$$

written in general linear method formulation has $s=1$ and is given as,

$$\left[\begin{array}{c} Y_1 \\ \hline y_m \\ hf(Y_1) \\ hf(y_{m-1}) \\ hf(y_{m-2}) \\ \vdots \\ hf(y_{m-k+1}) \end{array}\right] = \left[\begin{array}{c|cccccc} \beta_0 & 1 & \beta_1 & \beta_2 & \cdots & \beta_{k-1} & \beta_k \\ \hline \beta_0 & 1 & \beta_1 & \beta_2 & \cdots & \beta_{k-1} & \beta_k \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 \end{array}\right] \left[\begin{array}{c} hf(Y_1) \\ \hline y_{m-1} \\ hf(y_{m-1}) \\ hf(y_{m-2}) \\ hf(y_{m-3}) \\ \vdots \\ hf(y_{m-k}) \end{array}\right] \tag{14}$$

3.3. Two-Step Runge–Kutta Methods as General Linear Methods

The general form of a two step Runge–Kutta method with s stages is,

$$Y_i^{[m]} = (1-\alpha_i)y_m + \alpha_i y_{m-1} + h\sum_{j=1}^{s}[a_{ij}f(Y_j^{[m]}) + u_{ij}f(Y_j^{[m-1]})], \qquad i=1,\ldots,s,$$

$$y_{m+1} = (1-\vartheta)y_m + \vartheta y_{m-1} + h\sum_{j=1}^{s}[b_j f(Y_j^{[m]}) + v_j f(Y_j^{[m-1]})]. \tag{15}$$

Introducing a new variable z_m defined as,

$$z_m = \vartheta y_{m-1} + y_m + h\sum_{j=1}^{s} v_j f(Y_j^{m-1}). \tag{16}$$

This allows us to rewrite the equation for the internal stages in (15) as,

$$Y_i^{[m]} = \frac{1}{1+\vartheta} z_m + h\sum_{j=1}^{s} a_{ij} f(Y_j^{[m]}), \tag{17}$$

and update rule (15) as,

$$y_{m+1} = z_m - \vartheta y_m + h \sum_{j=1}^{s} b_j f(Y_j^{[m]}). \tag{18}$$

Inserting (18) into (16) we obtain,

$$z_{m+1} = z_m + h \sum_{j=1}^{s} (b_j + v_j) f(Y_j^{[m]}), \tag{19}$$

so that the resulting general linear method reads,

$$\left[\begin{array}{c} Y^{[m]} \\ \hline y^{[m+1]} \\ z^{[m+1]} \end{array}\right] = \left[\begin{array}{c|cc} A & 0 & \frac{1}{1+\vartheta} \\ \hline b^t & -\vartheta & 1 \\ b^t + v^t & 0 & 1 \end{array}\right] \left[\begin{array}{c} hf(Y^{[m]}) \\ \hline y^{[m]} \\ z^{[m]} \end{array}\right]. \tag{20}$$

4. G-symplecticity and control of parasitism

Symplectic one step methods preserve the quadratic invariants,

$$\langle y, y \rangle = y^T S y,$$

where S is a symmetric matrix. G-symplectic general linear methods preserve an extended version of the quadratic invariants given as,

$$\langle y^{[m]}, y^{[m]} \rangle_G = \langle y^{[m-1]}, y^{[m-1]} \rangle_G, \tag{21}$$

with $G \in \mathbb{R}^{r \times r}$ a symmetric matrix and

$$\langle y, z \rangle_G = \sum_{i,j=1}^{r} g_{ij} \langle y_i, z_j \rangle.$$

This is possible if and only if,

$$\begin{aligned} G &= V^T G V, \\ DU &= B^T G V, \\ DA + A^T D &= B^T G B. \end{aligned}$$

with $D \in \mathbb{R}^{s \times s}$ a diagonal matrix [3]. G-symplectic general linear methods suffer from parasitic instabilities similar to those encountered by standard linear multi-step methods. The reason is that the perturbation in parasitic components of the

numerical solution is amplified by the integration process.The parasitic growth parameter μ for a G-symplectic general linear method has been calculated in [8] and is obtained from the matrix product

$$BU = \begin{bmatrix} 1 & 0 \\ 0 & -\mu \end{bmatrix}.$$

The second order parasitic growth parameter has been calculated in [5]. Following [10], the parasitic growth parameter can be calculated by the formula,

$$\mu_i = (\xi_i)^{-1} w_i^* BU w_i, \tag{22}$$

where ξ_i is the i-th eigenvalue of V and w_i is the corresponding left eigenvector with $\xi_1 = 1$ and $\xi_i \neq 1$ for $2 \leq i \leq r$.

5. Projection Technique for General Linear Methods

Projection techniques are applicable to differential equations $y' = f(y(x))$ that reside on a manifold $\mathbf{N}$ given as,

$$\mathbf{N} = \{y; \psi(y) = 0\},$$

where $\psi(y)$ is an invariant of the given differential equation. Standard numerical methods produce approximate solutions that do not reside onto the manifold $\mathbf{N}$. Such methods can be combined with projection techniques, which ensure that the numerical solution stays on the manifold $\mathbf{N}$ at all times.
For general linear methods, standard projection technique has been implemented in [10]. The idea is to project only the first component of the output vector $y^{[m+1]}$ onto the manifold, namely by,

$$y_1^{[m+1]} = \tilde{y}_1^{[m+1]} + \frac{H(y_0) - H(\tilde{y}_1^{[m+1]})}{< \nabla H(\tilde{y}_1^{[m+1]}), \nabla H(\tilde{y}_1^{[m+1]}) >} \nabla H(\tilde{y}_1^{[m+1]}), \tag{23}$$

where $y_0 \in \mathbf{N}$ is the initial condition such that $\psi(y_0) = 0$, $\tilde{y}^{[m+1]} \notin \mathbf{N}$ is the approximate solution obtained by the general linear method and $\nabla H(y)$ is the gradient of $H(y)$.

6. Variational Integrators as General Linear Methods

6.1. Trapezoidal Rule

Let us recall the variational integrator based on trapezoidal rule (8) given as,

$$\nabla\alpha(q_m).\frac{q_{m+1}-q_{m-1}}{2h} = \frac{\alpha(q_{m+1})-\alpha(q_{m-1})}{2h} + \nabla H(q_m). \tag{24}$$

Let us define,

$$v_m = \frac{q_{m+1}-q_{m-1}}{2h}, \tag{25}$$

and

$$p = \alpha(q). \tag{26}$$

Then equation (24) can be rewritten as,

$$\frac{p_{m+1}-p_{m-1}}{2h} = \nabla\alpha(q_m)\cdot v_m - \nabla H(q_m). \tag{27}$$

The equations (25) and (27) are in fact an application of the central difference scheme to the differential equations given as,

$$\dot{q} = v, \tag{28}$$

$$\dot{p} = \nabla\alpha(q)\cdot v - \nabla H(q), \tag{29}$$

subject to (26). From (25) and (27), we have

$$q_{m+1} = q_{m-1} + 2hv_m, \tag{30}$$

$$p_{m+1} = p_{m-1} + 2h[\nabla\alpha(q_m)\cdot v_m - \nabla H(q_m)], \tag{31}$$

or in short,

$$y_{m+1} = y_{m-1} + 2hf(y_m, z_m), \tag{32}$$

where

$$y = (q,p)^T, \qquad f = (v, \nabla\alpha(q)\cdot v - \nabla H(q))^T. \tag{33}$$

It is interesting to note that the function f in (33) actually represents the right hand side of a Hamiltonian differential equation system corresponding to the given

Lagrangian. Evidently equation (32) is a multistep method, which can be written as a general linear method (14),

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cccc} 0 & 0 & 1 & 2 & 0 \\ \hline 0 & 0 & 1 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{array}\right]. \tag{34}$$

The method is G-symplectic with

$$G = \begin{bmatrix} 0 & 1 & 2 & 0 \\ 1 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad D = [2].$$

The parasitic growth parameter of (34) is computed by using (22) as $\mu_2 = -1.667$, so that the parasitic mode is unstable.

6.2. Mid-Point Rule

Let us recall the variational integrator based on mid-point rule (9) given as,

$$\begin{aligned} &\frac{1}{2}\nabla\alpha(\frac{q_m+q_{m+1}}{2})\cdot\frac{q_{m+1}-q_m}{h}+\frac{1}{2}\nabla\alpha(\frac{q_{m-1}+q_m}{2}).\frac{q_m-q_{m-1}}{h}= \\ &\frac{1}{h}[\alpha(\frac{q_m+q_{m+1}}{2})-\alpha(\frac{q_{m-1}+q_m}{2})]+\frac{1}{2}[\nabla H(\frac{q_m+q_{m+1}}{2})+\nabla H(\frac{q_{m-1}+q_m}{2})]. \end{aligned} \tag{35}$$

Upon defining,

$$v_{m+\frac{1}{2}} = \frac{q_{m+1}-q_m}{h}, \qquad \alpha(q_{m+\frac{1}{2}}) = p_{m+\frac{1}{2}} = \frac{p_m+p_{m+1}}{2},$$

equation (35) can be written as,

$$q_{m+\frac{1}{2}} = q_{m-\frac{1}{2}} + \frac{h}{2}[v_{m-\frac{1}{2}} + v_{m+\frac{1}{2}}], \tag{36}$$

$$\begin{aligned} p_{m+\frac{1}{2}} = p_{m-\frac{1}{2}} &+ \frac{h}{2}[\nabla\alpha(q_{m-\frac{1}{2}})\cdot v_{m-\frac{1}{2}} + \nabla\alpha(q_{m+\frac{1}{2}})\cdot v_{m+\frac{1}{2}}] \\ &- \frac{h}{2}[\nabla H(q_{m-\frac{1}{2}}) + \nabla H(q_{m+\frac{1}{2}})], \end{aligned} \tag{37}$$

and

$$q_{m+1} = q_{m-1} + h[v_{m-\frac{1}{2}} + v_{m+\frac{1}{2}}], \tag{38}$$

$$p_{m+1} = p_{m-1} + h[\nabla\alpha(q_{m-\frac{1}{2}}) \cdot v_{m-\frac{1}{2}} + \nabla\alpha(q_{m+\frac{1}{2}}) \cdot v_{m+\frac{1}{2}}] - h[\nabla H(q_{m-\frac{1}{2}}) + \nabla H(q_{m+\frac{1}{2}})], \tag{39}$$

or in short,

$$y_{m+\frac{1}{2}} = \frac{y_{m-1} + y_m}{2} + \frac{h}{2}[f(y_{m-\frac{1}{2}}) + f(y_{m+\frac{1}{2}})], \tag{40}$$

$$y_{m+1} = y_{m-1} + h[f(y_{m-\frac{1}{2}}) + f(y_{m+\frac{1}{2}})]. \tag{41}$$

The equation (41) is the two step Runge–Kutta method with just one internal stage (40), which can be written in general linear method form (20) as,

$$\left[\begin{array}{c|cc} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} 1/2 & 0 & 1/2 \\ \hline 1 & -1 & 1 \\ 2 & 0 & 1 \end{array}\right]. \tag{42}$$

The method is G-symplectic with

$$G = \begin{bmatrix} -2 & 1 \\ 1 & 1 \end{bmatrix}, \qquad D = [6].$$

The matrix V has two eigenvalues, -1 and 1 and the corresponding parasitic growth parameters are $\mu = 0$ and $\mu = 1$, so that the parasitic modes are stable. It is important to note that $p_m \neq \alpha(q_m)$, which is the root cause for the instability occurring in the algorithm.

7. Starting Algorithm

To find the value of q_{-1}, we use the position momentum form [15, 16]

$$p_m = -D_1 L_d(q_m, q_{m+1}), \tag{43}$$

$$p_{m+1} = D_2 L_d(q_m, q_{m+1}). \tag{44}$$

To obtain a relation between q_{-1}, q_0 and p_0, use the equation (44) as,

$$p_0 = D_2 L_d(q_{-1}, q_0),$$

but $p_0 = \alpha(q_0)$,

$$\implies \alpha(q_0) = D_2 L_d(q_{-1}, q_0).$$

8. Numerical Experiments

8.1. Lotka-Volterra Model

The Lotka–Volterra Model is often used in mathematical biology for modelling population growths of animal species. The dynamics of the growth of two species can be modelled by the following Lagrangian system,

$$L(q,\dot{q}) = (\frac{log\ q_2}{q_1} + q_2)\dot{q}_1 + q_1\dot{q}_2 - H(q),$$

with the Hamiltonian H given by,

$$H(q) = log\ q_1 - q_1 + 2log\ q_2 - q_2.$$

Here,

$$\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} = 0$$

An application of variational integrators using trapezoidal rule written as GLM (34) with initial condition $q_0 = (1,1)$ and step-size $h = 0.01$ yields the relative energy error in the Lotka–Volterra model as shown in Figure 1.

Figure 1 shows that the variational integrator (34) does not preserve the energy of the Lotka–Volterra model. We have calculated the relative energy error as follows,

$$\text{Error} = abs(H_e - H_n)/H_e,$$

where H_e is the exact energy at initial point and H_n is the approximate energy calculated at all numerical values. We then apply the projection technique (23) on GLM (34) and calculate the relative energy error again as shown in Figure 2.

Figure 2 shows that the variational integrator for degenerate Lagrangian of Lotka–Volterra model as GLM (34) with projection technique is preserving the energy very well.

An application of variational integrator using mid-point rule written as GLM (42) with initial condition $q_0 = (1,1)$ and step-size $h = 0.01$ yields the relative energy error in the Lotka–Volterra model as shown in Figure 3.

Figure 3 shows that the variational integrator (42) does not preserve the energy. We then apply the projection technique (23) on GLM (42) and calculate the relative energy error again as shown in Figure 4.

Figure 4 shows that the variational integrator for degenerate Lagrangian of Lotka–Volterra model as GLM (42) with projection technique is preserving the energy very well.

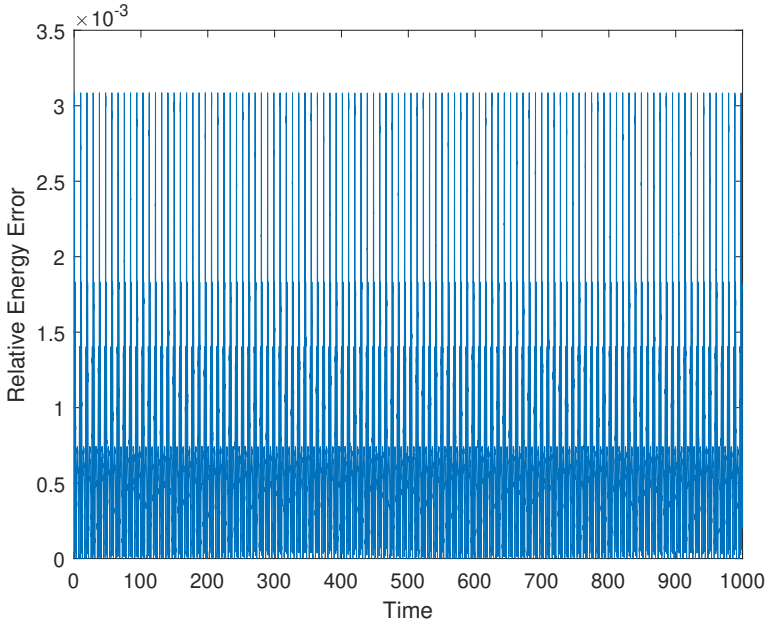

Figure 1 – The relative error in energy of the Lotka–Volterra model using GLM of variational integrator by trapezoidal rule without projection.

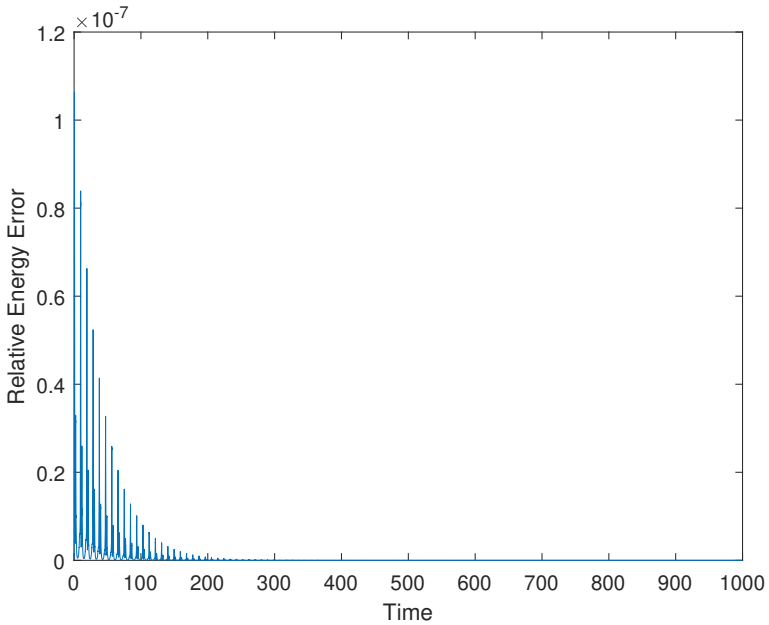

Figure 2 – The relative energy error in Lotka–Volterra model using GLM of variational integrator by trapezoidal rule with projection.

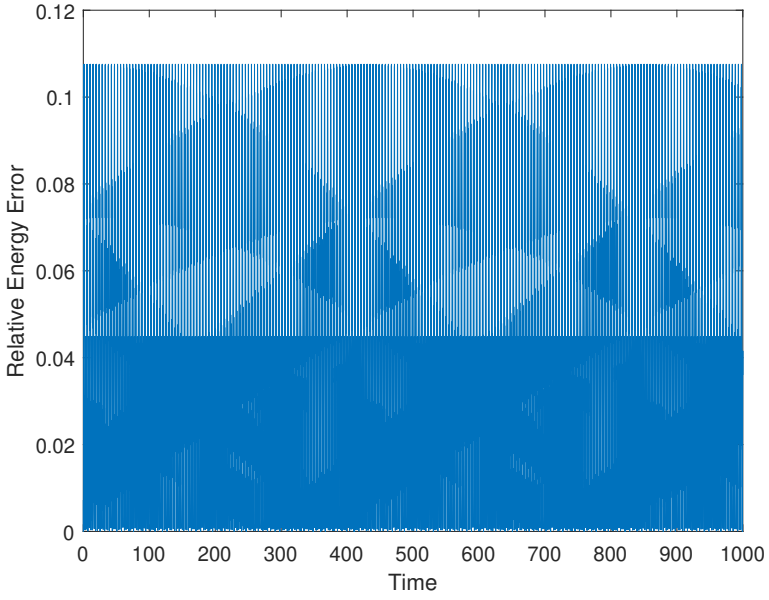

Figure 3 – The relative energy error in Lotka–Volterra model using GLM of variational integrator by mid-point rule without projection.

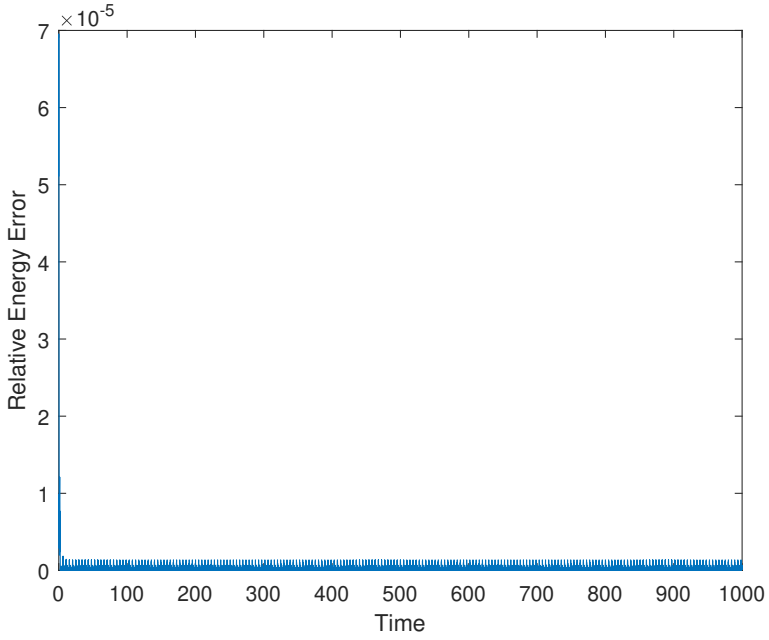

Figure 4 – The relative energy error in Lotka–Volterra model using GLM of variational integrator by mid-point rule with projection.

8.2. Pendulum

In order to shed light on variational integrator for degenerate Lagrangian system (9) expressed as a general linear method we consider non-linear pendulum whose Lagrangian is degenerate,

$$L(q,\dot{q}) = \begin{bmatrix} q^{[2]} & 0 \end{bmatrix} \begin{bmatrix} \dot{q}^{[1]} \\ \dot{q}^{[2]} \end{bmatrix} + cos(q^{[1]}) - \frac{(q^{[2]})^2}{2}. \tag{45}$$

An application of variational integrator using mid-point rule written as GLM (42) with initial condition $q_0 = (2.3, 0)$ and step-size $h = 0.01$ yields the relative energy error in the non-linear pendulum as shown in Figure 5.
Figure 5 shows that the variational integrator (42) does not preserve the energy. We then apply the projection technique (23) on GLM (42) and calculate the relative energy error again as shown in Figure 6.
Figure 6 shows that the variational integrator for degenerate Lagrangian of non-linear pendulum as GLM (42) with projection technique is preserving the energy very well.

9. Conclusions

We have written variational integrators for a class of degenerate Lagrangian system as general linear methods and have applied stabilisation mechanism for G-symplectic general linear methods to control the effect of parasitism.
We have demonstrated with some numerical examples, that these algorithms have excellent energy preserving properties for long time.

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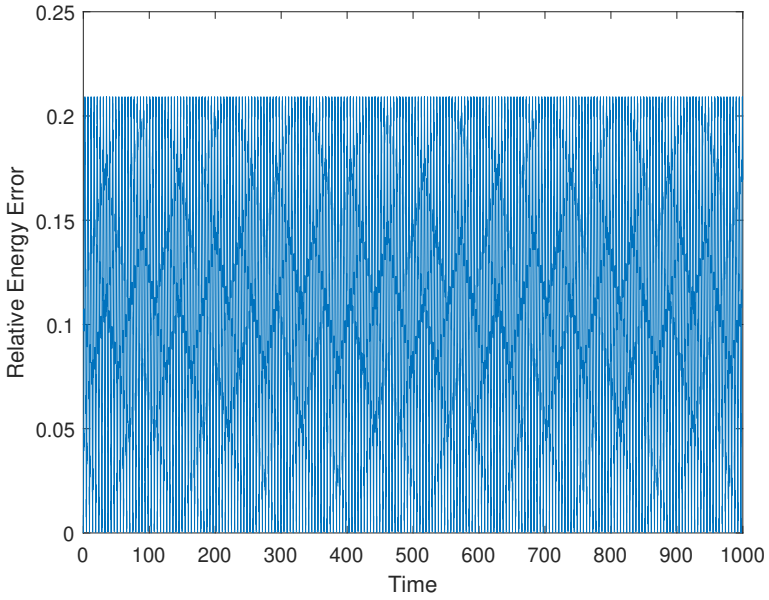

Figure 5 – The relative energy error in non-linear pendulum using GLM of variational integrator by mid-point rule without projection.

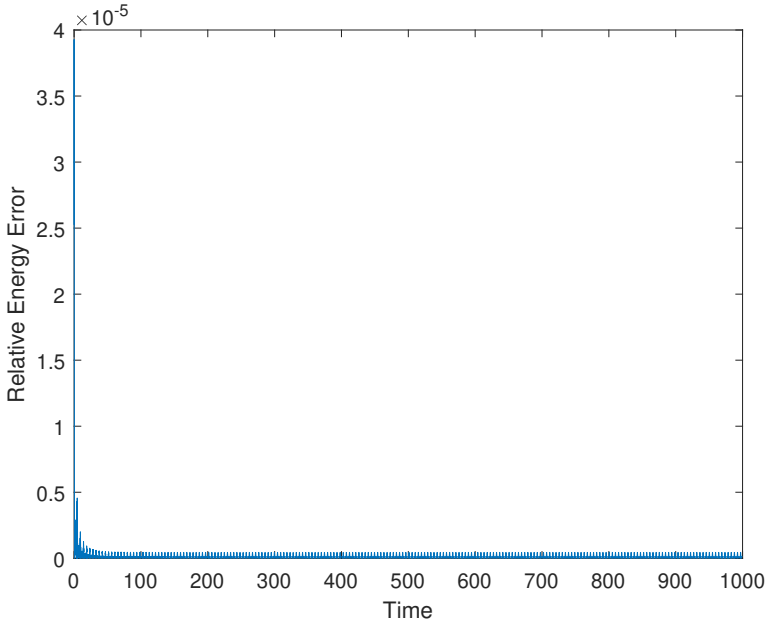

Figure 6 – The relative energy error in non-linear pendulum by using GLM of variational integrator by mid-point rule with projection.

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