ADAPTIVE VARIATIONAL INTEGRATORS

JEREMY SCHMITT AND MELVIN LEOK

Abstract. It is now well known that symplectic integrators lose many of their desirable properties when variable step sizes are used. The most common approach to combine adaptive step sizes and symplectic integrators involves the Poincaré transformation of the original Hamiltonian. In this article, we provide a framework for the construction of variational integrators using the Poincaré transformation. Since the transformed Hamiltonian is typically degenerate, the use of Hamiltonian variational integrators is required. This implies that the adaptive symplectic integrators resulting from applying a symplectic integrator to the transformed Hamilton's equations are best understood as coming from a type II or type III generating function, as opposed to a type I generating function. In addition, error analysis results and numerical examples are presented.

1. Introduction

Symplectic integrators are a class of geometric integrators that when applied to a Hamiltonian system yield a discrete approximation of the flow that preserves the symplectic 2-form (see [7]). The preservation of symplecticity results in the preservation of many qualitative aspects of the underlying dynamical system. In particular, when applied to conservative Hamiltonian systems, symplectic integrators show excellent long-time near-energy preservation. However, when symplectic integrators were first used in combination with variable time-steps, the near-energy preservation was lost and the integrators performed poorly (see [3], [5]). Backwards error analysis provided justification both for the excellent long-time near-energy preservation of symplectic integrators and for the poor performance experienced when using variable time-steps (see Chapter IX of [7]). Backward error analysis shows that symplectic integrators can be associated with a modified Hamiltonian in the form of a powers series in terms of the time-step. Changing the time-step results in a different modified Hamiltonian each time the time-step is varied. This is the source of the poor energy conservation. There has been a great effort to circumvent this problem, and there have been many successes. However, there has yet to be a unified general framework for constructing adaptive symplectic integrators. In this paper, we attempt to add to this effort by extending variable time-steps into the domain of variational integrators. Variational integrators are derived at the level of the variational principle, or equivalently, they are derived using generating functions. The Poincaré transformation results in a degeneracy that impedes the use of type I generating functions, but type II and type III generating functions have no difficulty with this degeneracy, which leads to the use of Hamiltonian variational integrators. The resulting framework yields variable time-step symplectic integrators that are analogous to those derived using the framework of [6], [15], but the theoretical framework at the level of the generating function has been expanded. After a brief introduction to variational integrators, we present a framework for variable time-step variational integrators, and contrast our method with existing work on the matter.

2. Variational Integrators

Variational integrators are symplectic integrators derived by discretizing Hamilton's principle, versus discretizing Hamilton's equations directly. As a result, variational integrators are symplectic, preserve many invariants and momentum maps, as well as having excellent long-time near-energy preservation (see [12]). Traditionally, variational integrators have focused on the type I generating function known as the discrete Lagrangian, $L_d : Q \times Q \mapsto \mathbb{R}$. The exact discrete Lagrangian

of the true flow of Hamilton's equations can be represented in both a variational form and in a boundary-value form. The latter is given by

$$L_d^E(q_0, q_1; h) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t))dt, \tag{1}$$

where $q_{01}(0) = q_0$, $q_{01}(h) = q_1$, and q_{01} satisfies the Euler–Lagrange equations over the time interval $[0, h]$. A variational integrator is defined by constructing an approximation to (1), $L_d : Q \times Q \mapsto \mathbb{R}$, and then applying the discrete Euler–Lagrange equations,

$$p_k = -D_1 L_d(q_k, q_{k+1}), \qquad p_{k+1} = D_2 L_d(q_k, q_{k+1}), \tag{2}$$

which implicitly define the integrator, $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$. The error analysis is greatly simplified via Theorem 2.3.1 of [12], which states that if a discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$, approximates the exact discrete Lagrangian, $L_d^E : Q \times Q \to \mathbb{R}$, to order r, i.e.,

$$L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) + \mathcal{O}(h^{r+1}),$$

then the discrete Hamiltonian map, $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, is order r accurate.

Many other properties of the integrator, such as symmetry of the method, can be determined by analyzing the associated discrete Lagrangian, as opposed to analyzing the integrator directly. More recently, variational integrators have been extended to the framework of type II and type III generating functions, commonly referred to as discrete Hamiltonians (see [9], [11]). Hamiltonian variational integrators are derived by discretizing Hamilton's phase space principle. The boundary-value formulation of the exact type II generating function of the time-h flow of Hamilton's equations is given by the exact discrete right Hamiltonian,

$$H_d^{+,E}(q_0, p_1; h) = p_1^T q_1 - \int_0^h \left[p(t)^T \dot{q}(t) - H(q(t), p(t))\right] dt, \tag{3}$$

where $(q(t), p(t))$ satisfy Hamilton's equations with boundary conditions $q(0) = q_0$ and $p(h) = p_1$. A type II Hamiltonian variational integrator is constructed by using an approximate discrete Hamiltonian, H_d^+, and applying the discrete right Hamilton's equations,

$$p_0 = D_1 H_d^+(q_0, p_1), \qquad q_1 = D_2 H_d^+(q_0, p_1),$$

which implicitly defines the integrator, $\tilde{F}_{H_d^+} : (q_0, p_0) \mapsto (q_1, p_1)$.

Various methods for constructing and analyzing Hamiltonian variational integrators can be found in [11], [16], and [17]. In particular, there is an analogous error analysis theorem as in the case of Lagrangian variational integrators. If a discrete right Hamiltonian, H_d^+, approximates the exact discrete right Hamiltonian, $H_d^{+,E}$, to order r, i.e.,

$$H_d^+(q_0, p_1; h) = H_d^{+,E}(q_0, p_1; h) + \mathcal{O}(h^{r+1}),$$

then the discrete right Hamilton's map, $\tilde{F}_{H_d^+} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, is order r accurate.

Hamiltonian and Lagrangian variational integrators are not always equivalent. In particular, it was shown in [16] that in some cases even when the Hamiltonian and Lagrangian integrators are analytically equivalent they can have different numerical properties. Even more to the point, Lagrangian variational integrators cannot always be constructed when the underlying Hamiltonian is degenerate, and in that situation, Hamiltonian variational integrators are the more natural choice. In the next section we examine a transformation commonly used to construct variable time-step symplectic integrators, which in most cases of interest results in a degenerate Hamiltonian. Our approach is to apply Hamiltonian variational integrators to the resulting transformed Hamiltonian system.

3. The Poincaré Transformation and Discrete Hamiltonians

Given a Hamiltonian, $H(q,p)$, and a desired transformation of time, $t \mapsto \tau$, given by $\frac{dt}{d\tau} = g(q,p)$, a new Hamiltonian system is given by the Poincaré transformation,

$$\bar{H}(\bar{q},\bar{p}) = g(q,p)\left(H(q,p) + p^t\right), \tag{4}$$

where $(\bar{q},\bar{p}) = \left(\begin{bmatrix} q \\ q^t \end{bmatrix}, \begin{bmatrix} p \\ p^t \end{bmatrix}\right)$. We will follow the common choice of setting $q^t = t$ and $p^t = -H(q(0),p(0))$, so that $\bar{H}(\bar{q},\bar{p}) = 0$ along all integral curves through $(q(0),p(0))$. The time t shall be referred to as the physical time, and τ as the fictive time. The corresponding Hamilton's equations are given by,

$$\dot{\bar{q}} = \begin{bmatrix} \nabla_p g(q,p) \\ 0 \end{bmatrix}\left(H(q,p)+p^t\right) + \begin{bmatrix} \frac{\partial H}{\partial p} \\ 1 \end{bmatrix} g(q,p), \qquad \dot{\bar{p}} = -\begin{bmatrix} \nabla_q g(q,p) \\ 0 \end{bmatrix}\left(H(q,p)+p^t\right) - \begin{bmatrix} \frac{\partial H}{\partial q} \\ 0 \end{bmatrix} g(q,p). \tag{5}$$

When the initial conditions are $(q(0),p(0))$, then $H(q,p)+p^t = 0$ and

$$\dot{\bar{q}} = \begin{bmatrix} g(q,p)\frac{\partial H}{\partial p} \\ g(q,p) \end{bmatrix}, \qquad \dot{\bar{p}} = \begin{bmatrix} -g(q,p)\frac{\partial H}{\partial q} \\ 0 \end{bmatrix}. \tag{6}$$

In general,

$$\frac{\partial^2 \bar{H}}{\partial \bar{p}^2} = \begin{bmatrix} \frac{\partial H}{\partial p}\nabla_p g(q,p)^T + g(q,p)\frac{\partial^2 H}{\partial p^2} + \nabla_p g(q,p)\frac{\partial H}{\partial p}^T & \nabla_p g(q,p) \\ \nabla_p g(q,p)^T & 0 \end{bmatrix},$$

which can be singular in many cases. Most of the papers cited here on variable time-step symplectic integrators focus exclusively on using a monitor function, g, that is only a function of position, in which case the resulting transformed Hamiltonian is degenerate and there is no corresponding Lagrangian formulation. Therefore, Hamiltonian variational integrators are the most general and natural way to derive variable time-step variational integrators.

The exact type II generating function for the transformed Hamiltonian is given by,

$$\bar{H}_d^{+,E}(\bar{q}_0,\bar{p}_1;h) = \bar{p}_1^T\bar{q}_1 - \int_0^h \left(\bar{p}(\tau)^T\dot{\bar{q}}(\tau) - \bar{H}(\bar{q}(\tau),\bar{p}(\tau))\right)d\tau, \tag{7}$$

where $(\bar{q}(\tau),\bar{p}(\tau))$ satisfy Hamilton's equations (6), with boundary conditions $\bar{q}(0) = \bar{q}_0$, $\bar{p}(h) = \bar{p}_1$.

The above exact discrete right Hamiltonian implicitly defines a symplectic map with respect to the symplectic form $\bar{\omega}(\bar{p}_k,\bar{q}_k)$ on $T^*\bar{Q}$ via the discrete Legendre transforms given by,

$$\bar{p}_0 = \frac{\partial \bar{H}_d^{+,E}}{\partial \bar{q}_0}, \qquad \bar{q}_1 = \frac{\partial \bar{H}_d^{+,E}}{\partial \bar{p}_1}.$$

Our approach is to construct Hamiltonian variational integrators by using a discrete right Hamiltonian, $\bar{H}_d^+$, that approximates (7) to order r, then the resulting integrator will be a variable time-step symplectic integrator. It is important to note that this method will be symplectic in two different ways. It will be symplectic both with respect to the symplectic form $d\bar{p}\wedge d\bar{q}$ and with respect to the symplectic form $dp\wedge dq$. Since p_t is constant(i.e. $p_0^t = \frac{\partial \bar{H}_d^+}{\partial q_0^t} = p_1^t$), the symplectic form in generalized coordinates is given by

$$\begin{aligned}\bar{\omega}(\bar{p}_k,\bar{q}_k) &= d\bar{p}_k\wedge d\bar{q}_k \\ &= \sum_{i=1}^{n+1} d\bar{p}_{k,i}\wedge d\bar{q}_{k,i} \\ &= \sum_{i=1}^{n} dp_{k,i}\wedge dq_{k,i} + dp_k^t\wedge dq_k^t\end{aligned}$$

$$= \sum_{i=1}^{n} dp_{k,i} \wedge dq_{k,i}$$
$$= \omega(p_k, q_k).$$

A symplectic variable time-step method was proposed independently in [6] and [15], which applied a symplectic integrator to the Hamiltonian system resulting from the Poincaré transformation. In [6], it is noted that one of the first applications of the Poincaré transformation was by Levi-Civita, who applied it to the three-body problem. A more in-depth discussion of such time transformations can be found in [18]. There has been further work using this transformation in papers such as [1] and [2], which focus on developing symplectic, explicit, splitting methods with variable time-steps.

Our approach is to discretize the type II generating function for the flow of Hamilton's equations, where the Hamiltonian is given by the Poincaré transformation. Therefore, we are constructing variational integrators, and in particular Hamiltonian variational integrators (see [9], [11]). This approach works seamlessly with existing methods and theorems of Hamiltonian variational integrators, but now the system under consideration is the transformed Hamiltonian system resulting from the Poincaré transformation. The methods of [6] and [15] include the possibility of applying a given variational integrator to the transformed differential equations. Our approach gives a framework for constructing variational integrators at the level of the generating function by using the Poincaré transformed discrete right Hamiltonian. In most cases, these two approaches will produce equivalent integrators, but our new approach allows for the method to analyzed at the level of the generating function, and indicates that most such symplectic methods are best interpreted as coming from a type II or III generating function, as opposed to a type I generating function.

Remark. *Other approaches to variable time-step variational integrators can be found in [8], [13] and [14]. In particular, [8] is inspired by the result of Ge and Marsden ([4]), which states that constant time-step symplectic integrators of autonomous Hamiltonian systems cannot exactly conserve the energy unless it agrees with the exact flow map up to a time reparametrization. Therefore, they sought a variable time-step energy-conserving symplectic integrator in an expanded non-autonomous system. However, symplecticity is with respect to the space-time symplectic form $dp \wedge dq + dH \wedge dt$. The time-step is determined by enforcing discrete energy conservation, which arises as a consequence of the fact that energy is the Noether quantity associated with time translational symmetry. An extended Hamiltonian is used that is similar in spirit to the Poincaré transformation. An approach that builds off this idea and space-time symplecticity was presented in [14], and a less constrained choice of time-step was allowed.*

In [13], adaptive variational integrators are constructed using a transformation of the Lagrangian, which is motivated by the Poincaré transformation, but it is not equivalent. The lack of equivalence is not surprising, since the Hamiltonian given by the Poincaré transformation is degenerate for their choice of monitor functions. As a consequence, the phase space path is not preserved.

4. Variational Error Analysis

The standard error analysis theorem for Hamiltonian variational integrators assumes a non-degenerate Hamiltonian, i.e., $\det(\frac{\partial^2 \bar{H}}{\partial \bar{p}^2}) \neq 0$ (see [16]). The non-degeneracy implies that the usual implicit function theorem can be applied to the discrete right Hamilton's equations. In particular, the proof of the error analysis theorem relies upon the following lemma, which follows from the implicit function theorem.

Lemma 1. *Let $f_1, g_1, e_1, f_2, g_2, e_2 \in C^r$ be such that*

$$f_1(x,h) = g_1(x,h) + h^{r+1} e_1(x,h),$$
$$f_2(x,h) = g_2(x,h) + h^{r+1} e_2(x,h).$$

Then, there exists functions e_{12} and $\bar{e}_1$ bounded on compact sets such that

$$f_2(f_1(x,h),h) = g_2(g_1(x,h),h) + h^{r+1}e_{12}(g_1(x,h),h),$$
$$f_1^{-1}(y) = g_1^{-1}(y) + h^{r+1}\bar{e}_1(y).$$

Combining this lemma with the discrete right Hamiltonian map,

$$\tilde{F}_{H_d^+}(q_0,p_0) = \mathbb{F}^+H_d^+ \circ (\mathbb{F}^-H_d^+)^{-1}(q_0,p_0) = (q_1,p_1),$$

ensures the order of accuracy of the integrator is at least of the order to which H_d^+ approximates $H_d^{+,E}$. Since the usual implicit function theorem does not apply, we need to justify the invertibility of $\mathbb{F}^-H_d^+$, which comes down to whether $\bar{p}_0 = D_1\bar{H}_d^+(\bar{q}_0,\bar{p}_1;h)$ can be solved for $\bar{p}_1$.

We assume the original Hamiltonian, $H(q,p)$, is nondegenerate. Then, we will show that the exact discrete right Hamiltonian can be reduced to a particular form and the extended variables p_1^t and q_1^t can be solved for explicitly. As a result, the implicit function theorem is not needed with respect to these variables. Hamilton's equations of the transformed Hamiltonian, $\bar{H}(\bar{q},\bar{p}) = g(q,p)\left(H(q,p)+p^t\right)$, are

$$\dot{\bar{q}} = \begin{bmatrix}\nabla_p g(q,p)\\ 0\end{bmatrix}\left(H(q,p)+p^t\right) + \begin{bmatrix}\frac{\partial H}{\partial p}\\ 1\end{bmatrix} g(q,p), \qquad \dot{\bar{p}} = -\begin{bmatrix}\nabla_q g(q,p)\\ 0\end{bmatrix}\left(H(q,p)+p^t\right) - \begin{bmatrix}\frac{\partial H}{\partial q}\\ 0\end{bmatrix} g(q,p).$$

The corresponding exact discrete right Hamiltonian is of the form

$$\begin{aligned}\bar{H}_d^{+,E}(\bar{q}_0,\bar{p}_1;h) &= \bar{p}_1^T\bar{q}_1 - \int_0^h \left(\bar{p}(\tau)^T\dot{\bar{q}}(\tau) - \bar{H}(\bar{q}(\tau),\bar{p}(\tau))\right)d\tau\\ &= p_1^Tq_1 + p_1^tq_1^t - \int_0^h \big(p(\tau)^T\dot{q}(\tau) + p^t(\tau)g(q(\tau),p(\tau)) - g(q(\tau),p(\tau))p^t(\tau)\\ &\qquad\qquad - g(q(\tau),p(\tau))H(q(\tau),p(\tau))\big)\,d\tau\\ &= p_1^Tq_1 + p_1^tq_1^t - \int_0^h \left(p(\tau)^T\dot{q}(\tau) - g(q(\tau),p(\tau))H(q(\tau),p(\tau))\right)d\tau.\end{aligned}$$

As a result, only one part of this exact discrete right Hamiltonian requires approximations of the extended variable q^t and p^t. Furthermore, since $\dot{p}^t = 0$ this implies $p_1^t = p_0^t$. Now, let $\bar{H}_d^+(\bar{q}_0,\bar{p}_1;h)$ be an approximation to the exact discrete right Hamiltonian of the form

$$\bar{H}_d^+(\bar{q}_0,\bar{p}_1;h) = p_1^T\hat{q}_1(q_0,p_1;h) + p_1^t\hat{q}_1^t(q_0^t,q_0,p_1;h) - I(q_0,p_1;h),$$

where $\hat{\cdot}$ denotes an approximated value and $I(q_0,p_1;h)$ is an approximation of

$$\int_0^h \left(p(\tau)^T\dot{q}(\tau) - g(q(\tau),p(\tau))H(q(\tau),p(\tau))\right)d\tau.$$

Then, the discrete right Legendre transforms, $\bar{p}_0 = D_1\bar{H}_d^+(\bar{q}_0,\bar{p}_1;h)$ and $\bar{q}_1 = D_2\bar{H}_d^+(\bar{q}_0,\bar{p}_1;h)$, give the following explicit relations for p_1^t and q_1^t,

$$\begin{bmatrix}p_0\\ p_0^t\end{bmatrix} = \begin{bmatrix}\frac{\partial\hat{q}_1}{\partial q_0}^T p_1 + p_1^t\frac{\partial\hat{q}_1^t}{\partial q_0} - \frac{\partial I}{\partial q_0}\\ \frac{\partial\hat{q}_1^t}{\partial q_0^t}p_1^t\end{bmatrix},$$
$$\begin{bmatrix}q_1\\ q_1^t\end{bmatrix} = \begin{bmatrix}\hat{q}_1 + \frac{\partial\hat{q}_1}{\partial p_1}^T p_1 + \frac{\partial\hat{q}_1}{\partial p_1}^T p_1^t - \frac{\partial I}{\partial p_1}\\ \hat{q}_1^t\end{bmatrix}.$$

Now, since the analytic solution satisfies $p_1^t = p_0^t$, there is no need to approximate p_1^t. Therefore, $\frac{\partial\hat{q}_1^t}{\partial q_0^t} = 1$, and p_1^t is given independently of the other values. The upshot is a system that can be solved by first setting $p_1^t = p_0^t$, then implicity solving for p_1 in terms of (q_0^t,q_0,p_1^t,p_1), explicitly

solving for q_1 and finally explictly solving for q_1^t. Since p_1 is not determined by q_1^t, the implicit function theorem is simply needed for finding p_1. Therefore, we need $\det(\frac{\partial^2 \bar{H}}{\partial p^2}) \neq 0$, which is the same as $\det(\frac{\partial H}{\partial p}\nabla_p g(q,p)^T + g(q,p)\frac{\partial^2 H}{\partial p^2} + \nabla_p g(q,p)\frac{\partial H}{\partial p}^T) \neq 0$. Note this holds for nondegenerate Hamiltonians H and p-independent monitor functions. The result that we have established is summarized in the following theorem.

Theorem 1. *Given a nondegenerate Hamiltonian H, and a monitor function $g \in C^1([0,h])$, such that $\det(\frac{\partial H}{\partial p}\nabla_p g(q,p)^T + g(q,p)\frac{\partial^2 H}{\partial p^2} + \nabla_p g(q,p)\frac{\partial H}{\partial p}^T) \neq 0$. Then, if the discrete right Hamiltonian $\bar{H}_d^+$, approximates the exact discrete right Hamiltonian $\bar{H}_d^{+,E}$, to order r, i.e.,*

$$\bar{H}_d^+(\bar{q}_0, \bar{p}_1; h) = \bar{H}_d^{+,E}(\bar{q}_0, \bar{p}_1; h) + \mathcal{O}(h^{r+1}),$$

then the discrete right Hamilton's map $\tilde{F}_{\bar{H}_d^+} : (\bar{q}_k, \bar{p}_k) \mapsto (\bar{q}_{k+1}, \bar{p}_{k+1})$, viewed as a one-step method, is order r accurate.

5. Adaptive Hamiltonian Taylor Variational Integrators

We will demonstrate the approach using Hamiltonian Taylor variational integrators (see [17]), which are constructed as follows:

(i) Construct a r-order Taylor expansion,$\Psi_h^{(r)}$, on the cotangent bundle, $T^*\bar{Q}$, and solve for $\tilde{\bar{p}}_0$,

$$\bar{p}_1 = \pi_{T^*\bar{Q}} \circ \Psi_h^{(r)}(\bar{q}_0, \tilde{\bar{p}}_0),$$

where $\pi_{T^*\bar{Q}} : (\bar{q}, \bar{p}) \mapsto \bar{p}$.

(ii) Pick a quadrature rule of order s with quadrature weights and nodes given by (b_i, c_i) for $i = 1, \ldots, m$.

(iii) Use a r-order Taylor method to generate approximations of $(\bar{q}(t), \bar{p}(t))$ at the quadrature nodes,

$$(\bar{q}_{c_i}, \bar{p}_{c_i}) = \Psi_{c_i h}^{(r)}(\bar{q}_0, \tilde{\bar{p}}_0),$$

and use a $(r+1)$-order Taylor method on the configuration manifold to generate the approximation to the boundary term $\bar{q}_1$,

$$\tilde{\bar{q}}_1 = \pi_{\bar{Q}} \circ \Psi_h^{(r+1)}(\bar{q}_0, \tilde{\bar{p}}_0).$$

(iv) Use the quadrature rule and approximate boundary term, $\tilde{\bar{q}}_1$, to construct the discrete right Hamiltonian of order $\min(r+1, s)$,

$$\bar{H}_d^+(\bar{q}_0, \bar{p}_1; h) = \bar{p}_1^T \tilde{\bar{q}}_1 - h \sum_{i=1}^{m} \left[\bar{p}_{c_i}^T \dot{\bar{q}}_{c_i} - \bar{H}\left(\Psi_{c_i h}^{(r)}(\bar{q}_0, \tilde{\bar{p}}_0) \right) \right].$$

(v) The method is implicitly defined by the implicit discrete right Hamilton's equations,

$$\bar{q}_1 = D_2 \bar{H}_d^+(\bar{q}_0, \bar{p}_1), \qquad \bar{p}_0 = D_1 \bar{H}_d^+(\bar{q}_0, \bar{p}_1). \tag{8}$$

For a lucid exposition, we will at first assume $g(q,p) = g(q)$ and $H(q,p) = \frac{1}{2}p^T M^{-1} p + V(q)$. Consider the discrete right Hamiltonian given by approximating $\bar{q}_1$ with a first-order Taylor method about $\bar{q}_0$, approximating $\bar{p}_0$ with a zeroth-order Taylor expansion about $\bar{p}_0$, and using the rectangular quadrature rule about the initial point, which yields

$$\bar{H}_d^+ = p_1^T(q_0 + hg(q_0)M^{-1}p_1) + p_1^t(q_0^t + hg(q_0)) - hg(q_0)\left[\frac{1}{2}p_1^T M^{-1} p_1 - V(q_0)\right]. \tag{9}$$

The corresponding variational integrator is given by,

$$\bar{p}_1 = \begin{bmatrix} p_0 - hg(q_0)\nabla V(q_0) - h\nabla g(q_0)\left(\frac{1}{2}p_1^T M^{-1} p_1 + V(q_0) + p_0^t\right) \\ p_0^t \end{bmatrix}, \tag{10}$$

$$\bar{q}_1 = \begin{bmatrix} q_0 + hg(q_0)M^{-1}p_1 \\ q_0^t + hg(q_0) \end{bmatrix}. \tag{11}$$

The resulting integrator is merely symplectic Euler-B applied to the transformed Hamiltonian system,

$$\bar{q}_1 = \bar{q}_0 + h\frac{\partial \bar{H}(\bar{q}_0, \bar{p}_1)}{\partial \bar{p}},$$

$$\bar{p}_1 = \bar{p}_0 - h\frac{\partial \bar{H}(\bar{q}_0, \bar{p}_1)}{\partial \bar{q}}.$$

In fact, this is precisely the adaptive symplectic integrator first proposed in [6] and also presented on page 254 of [10]. Most existing symplectic integrators can be interpreted as variational integrators, but there are also new methods that are most naturally derived as variational integrators. We will also consider a fourth-order Hamiltonian variational integrator recently developed in [17], which is distinct from any existing symplectic method.

One of the most important aspects of implementing a variable time-step symplectic integrator of this form is a well chosen monitor function, $g(q)$. We need g to be positive-definite, so that we never stall or march backward in time. Noting that the above integrator is first-order, a natural choice is to use the second-order truncation error given by $-\frac{(q_1^t - q_0^t)^2}{2}M^{-1}\nabla V(q_0)$. Let tol be some desired level of accuracy, then one choice for g would be,

$$g(q_0) = \frac{tol}{\|\frac{(q_1^t - q_0^t)^2}{2}g(q_0)M^{-1}\nabla V(q_0)\|}. \tag{12}$$

Noting that $q_1^t - q_0^t = hg(q_0)$, we have,

$$g(q_0) = \frac{tol}{\|\frac{h^2 g(q_0)^3}{2}M^{-1}\nabla V(q_0)\|}, \tag{13}$$

which yields,

$$g(q_0) = \left(\frac{tol}{\|\frac{h^2}{2}M^{-1}\nabla V(q_0)\|}\right)^{\frac{1}{4}}. \tag{14}$$

This justifies our choice for g as,

$$g(q_0) = \frac{tol}{\|\frac{h^2}{2}M^{-1}\nabla V(q_0)\|}, \tag{15}$$

which achieves an error which is comparable to the chosen value of tol.

Alternative choices of g, proposed in [6], include the p-independent arclength parameterization given by,

$$g(q) = (2(H_0 - V(q)) + \nabla V(q)^T M^{-1}\nabla V(q))^{-\frac{1}{2}}, \tag{16}$$

and a choice particular to Kepler's two-body problem,

$$g(q) = q^T q, \tag{17}$$

which is motivated by Kepler's second law, which states that a line segment joining the two bodies sweeps out equal areas during equal intervals of time.

We have tested the algorithm given by (11) on Kepler's planar two-body problem, with an eccentricity of 0.9, using the three choices of g given by (15), (16), and (17). Of these three choices,

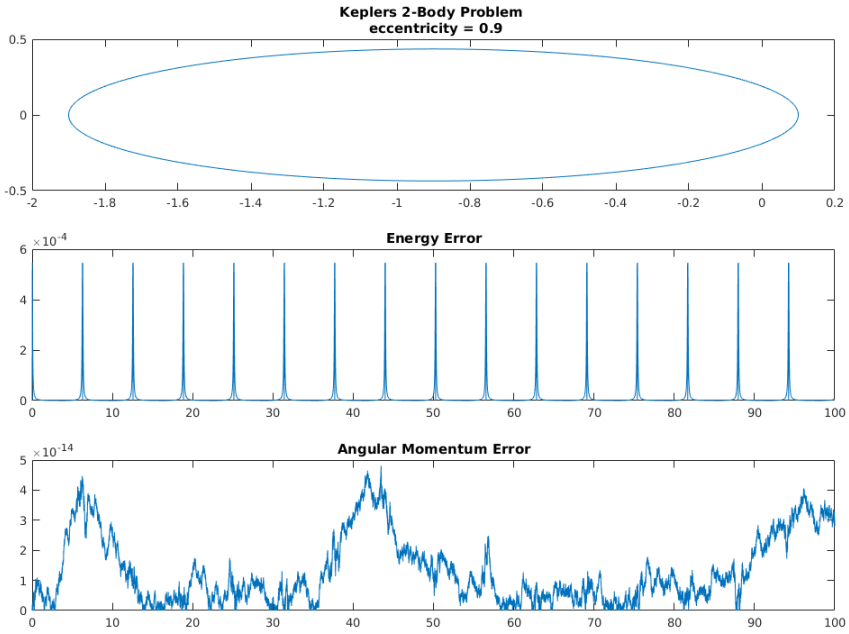

FIGURE 1. Symplectic Euler-B was applied to Kepler's planar two-body problem over a time interval of $[0, 100]$ with an eccentricity of 0.9. A time-step of $h = 0.00001$ was used, and it took 10,000,000 steps. Global error $= 5.5 \cdot 10^{-4}$.

(17) is particular to Kepler's two-body problem, while (15) and (16) are more general choices. However, since (15) is based on the truncation error, the cost of computing this function will increase as the order of the method increases. In contrast, (16) is independent of the order. Simulations using Kepler's two-body problem with an eccentricity of 0.9 over a time interval of $[0, 1000]$ were run using the three different choices of g and the usual symplectic Euler-B. Results indicate that symplectic Euler-B takes the most steps and computational time to achieve a level of accuracy around 10^{-5}. To achieve a level of accuracy around 10^{-5}, the choice of the truncation error monitor function, (15), resulted in the least number of steps, and the second lowest computational time. The lowest computational time belonged to (17), but it used significantly more steps than (15). The lower computational cost can be attributed to the cheaper evaluation cost of the monitor function and its derivative. Finally, the monitor function (16) required the most steps and computational time of the adaptive algorithms, but it is still a good choice in general given its broad applicability. See Figures 1, 2, and 3.

Next, we consider the fourth-order Hamiltonian Taylor variational integrator constructed using Taylor methods up to order 3 and Simpson's quadrature rule. We will now drop the assumption of p-independent monitor functions and consider $g(q, p)$. The following monitor functions were considered,

$$g(q) = \left(q^T q\right)^{\gamma} \text{ for } \gamma = \frac{1}{2}, 1 \tag{18}$$

$$g(q) = \left(2(H_0 - V(q)) + \nabla V(q)^T M^{-1} \nabla V(q)\right)^{-\frac{1}{2}} \tag{19}$$

$$g(q, p) = \|p^t - L(q, M^{-1}p)\|_2^{-1} \tag{20}$$

The monitor function (20) was originally intended to be $\|p^t + H(q, p)\|_2^{-1}$, but an accidental error led to the conclusion that (20) is the better choice. We will discuss the shortcomings of using

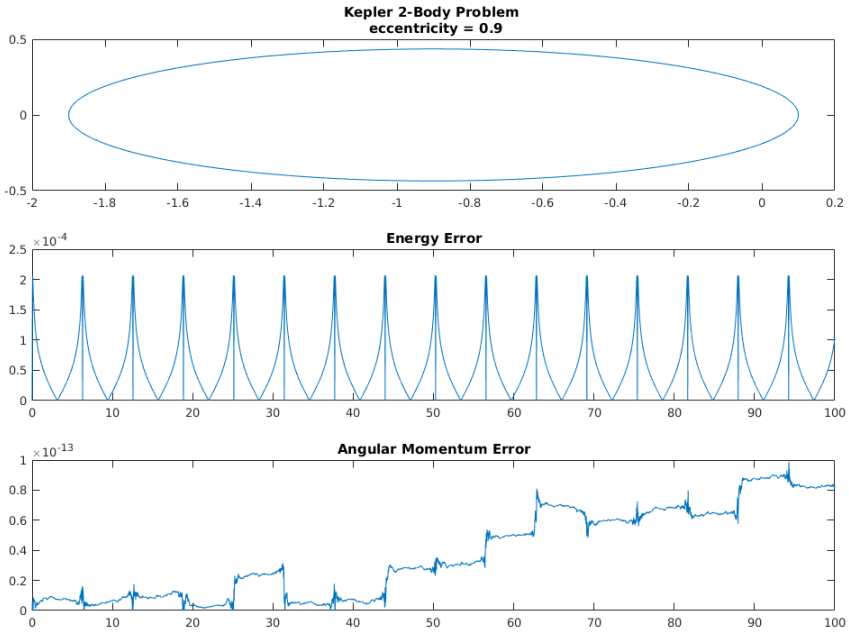

FIGURE 2. The adaptive algorithm with monitor function (15) applied to Kepler's planar two-body problem over a time interval of $[0, 100]$ with an eccentricity of 0.9. The tolerance was set to 10^{-5} and it took 1,123,116 steps. Global error $= 4.2 \cdot 10^{-5}$.

the inverse energy error in the next paragraph. Note that $\|L(q, M^{-1}p)\|_2^{-1}$ also performs decently, but the addition of $p^t = -H(q_0, p_0)$ showed noticeable improvement. It was noted in [6] that the inverse Lagrangian has been considered as a possible choice for g in the Poincaré transformation, but not in the framework of symplectic integration. While the choice of (18) was generally the most efficient, (20) was very close in terms of efficiency and offers a more general monitor function. This also implies that efficiency is not limited to only q or p-independent monitor functions. However, various attempts to construct seperable transformed Hamiltonians (see [1], [2]) required the use of q or p-independent monitor functions, so this is where such monitor functions are most useful.

The truncation error monitor function, (15), performed quite well for first-order methods, and this motivated the choice of using Taylor variational integrators, since derivatives would be readily available. However, its success cannot as easily be applied to higher-order methods. This is due to the fact that for higher-order truncation errors, one obtains an implicit differential-algebraic definition of the monitor function. This deviates from the first-order case, where the monitor function can be solved for explicitly. Another seemingly natural choice for the monitor function is the inverse of the energy error. However, Taylor variational integrators are constructed using Taylor expansions about the initial point, and consequently the monitor function is largely evaluated about the initial point. If the initial point is at a particularly tricky part of the dynamics and requires a small first step, then the energy error at the first step will not reflect this, since initially the energy error is zero. In contrast, the inverse Lagrangian will be small at an initial point that requires a small first step. The inverse energy error may work well for methods that primarily evaluate the energy error at the end point rather than the initial point.

Additionally, it is often advantageous to bound the time-step below or above. As noted on page 248 of [10], this can be done by setting $a = \frac{\Delta t_{\min}}{\Delta \tau}$ and $b = \frac{\Delta t_{\max}}{\Delta \tau}$, then defining the new monitor

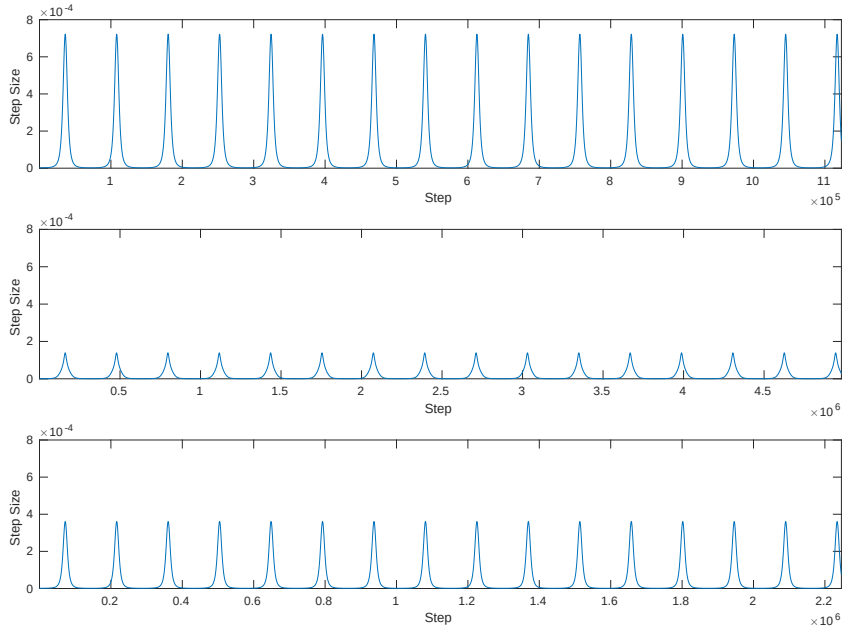

FIGURE 3. The time-steps taken for the various choices of monitor functions. The top plot corresponds to (15), the middle plot corresponds to (16), and the bottom plot corresponds to (17). All of the monitor functions appear to increase and decrease time-step at the same points along the trajectory, but clearly (15) allowed for the larger steps to be taken.

function as,

$$\hat{g} = b\frac{g+a}{g+b}. \tag{21}$$

Note that for methods such as the Taylor variational integrator, bounding $g(q,p)$ does bound the step-size, but not directly (see the tables below for a comparison of bounds, computationals time, steps, and error).

Compared to non-adaptive variational integrators, the adaptive methods showed a significant gain in efficiency for Kepler's 2-body planar problem with high eccentricity, while low eccentricity models do not need nor do they benefit from adaptivity. A Hamiltonian dynamical system with regions of high curvature in the vector field and its norm will in general benefit from an adaptive scheme such as the one outlined here.

Kepler Planar two-Body Problem, Eccentricity = 0.9										
Method	Monitor	h	min Step	max Step	min g	max g	Energy Error	Global Error	Steps	Time
HTVI4	Gamma	0.1	0.0020	0.2493	0.01	8	1.43E-05	7.09E-06	181	26.9
HTVI4	Energy	0.1	0.0051	0.1809	0.0001	2	1.93E-06	4.76E-06	146	28.3
HTVI4	Arclength	0.1	0.0040	0.1458	0.003	0.3	1.10E-04	3.69E-05	185	70.2
HTVI4	-	0.0025	0.0025	0.0025	-	-	2.50E-06	2.89E-05	4000	120

6. CONCLUSION

Due to the degeneracy of the Hamiltonian, adaptive variational integrators based on the Poincaré transformation should be constructed using discrete Hamiltonians, which are type II or III generating functions. This has potential implications for the numerical properties of such integrators,

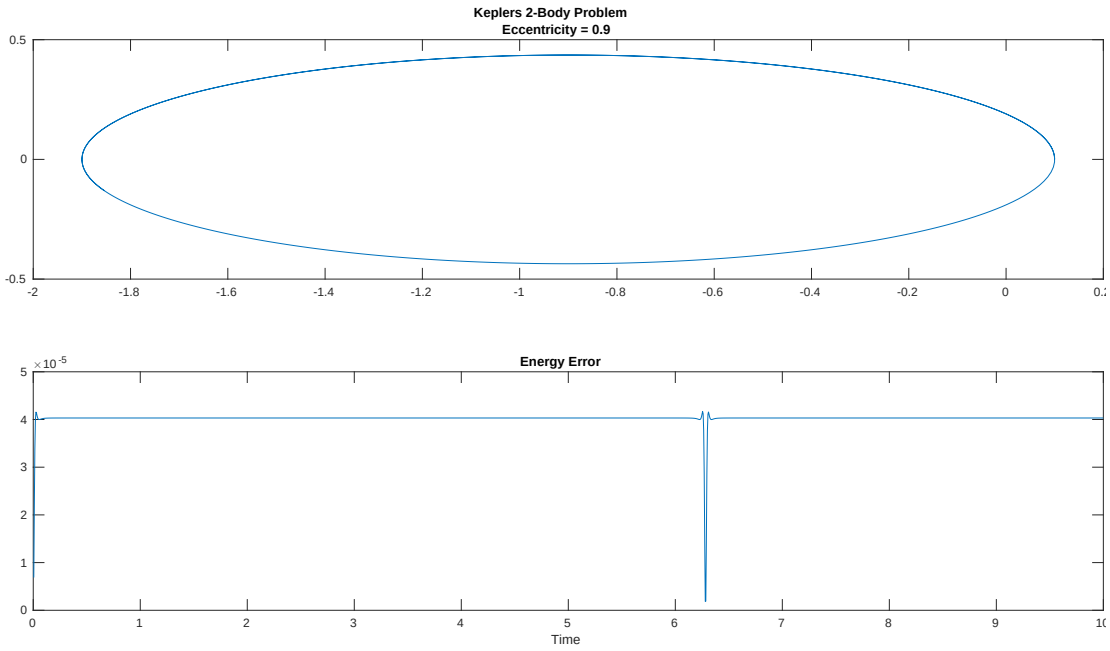

FIGURE 4. The fourth-order Hamiltonian Taylor variational integrator with a time-step of $h = 0.005$. It was applied to Kepler's planar two-body problem over a time interval of $[0, 10]$ with an eccentricity of 0.9, and the method required 2000 steps to achieve a global error of around $6.2 \cdot 10^{-5}$.

Kepler Planar two-Body Problem, Eccentricity = 0.99										
Method	Monitor $g(q,p)$	h	min Step	max Step	min g	max g	Energy Error	Global Error	Steps	Time
HTVI4	Gamma	0.1	0.00006	0.2648	0.0005	8	4.88E-05	5.60E-06	372	49.3
HTVI4	Energy	0.03	0.00015	0.1462	1E-6	5	9.13E-06	4.63E-06	383	58.4
HTVI4	Arclength	0.1	0.00005	0.1379	0.0008	10	1.31E-05	1.49E-05	691	146.0
HTVI4	-	0.0005	0.0005	0.0005	-	-	1.38E-01	7.83E-01	20000	525.2
SV	-	5E-7	5E-7	5E-7	-	-	3.34E-06	2.68E-05	2E7	189.2

and might explain why there has only been a limited amount of work on the construction of adaptive variational integrators based on the traditional Lagrangian perspective. The efficiency of the resulting integrator is largely based upon a proper choice of the monitor function g, and more research is needed to find a general choice of g that maintains a decent level of efficiency. Galerkin variational integrators are likely to be a more promising choice than Taylor variational integrators, since the cost of evaluating the monitor function and its derivatives should be lower. In addition, the Galerkin approximation scheme may help inform a better choice of monitor function, due to the extensive literature on efficient *a posteriori* error estimation. *A posteriori* error estimation, in general, would be a nice addition to give some guarantees on global accuracy.

ACKNOWLEDGEMENTS

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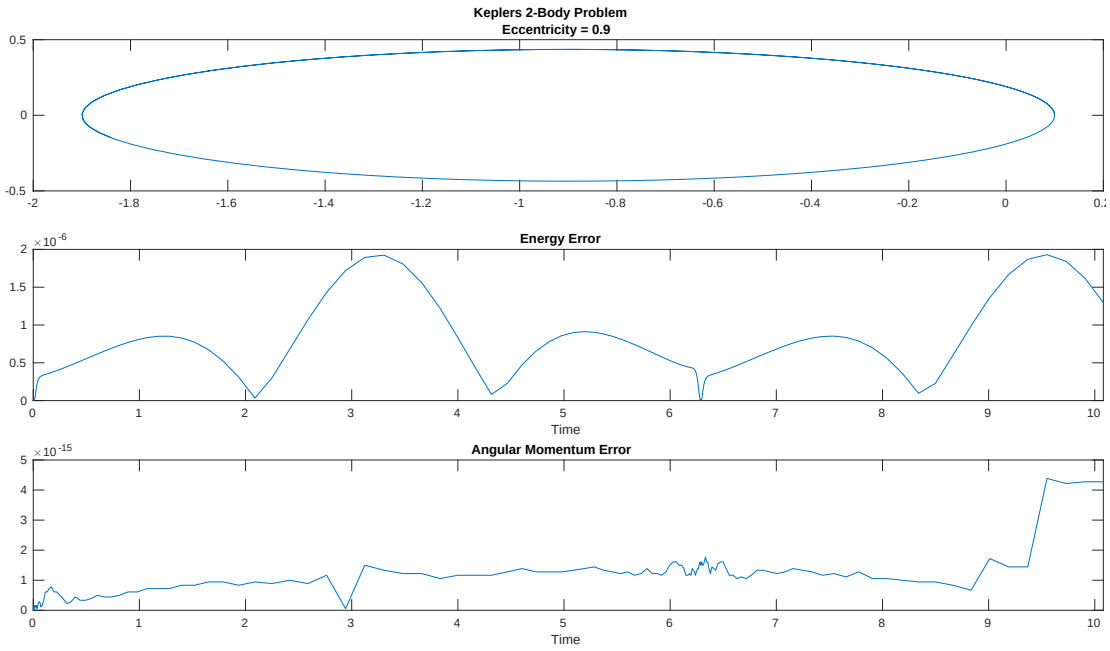

FIGURE 5. The adaptive fourth-order Hamiltonian Taylor variational integrator using the monitor function (20). It was applied to Kepler's planar two-body problem over a time interval of $[0, 10]$ with an eccentricity of 0.9, and it took 146 steps and had a global error $= 4.76 \cdot 10^{-6}$.

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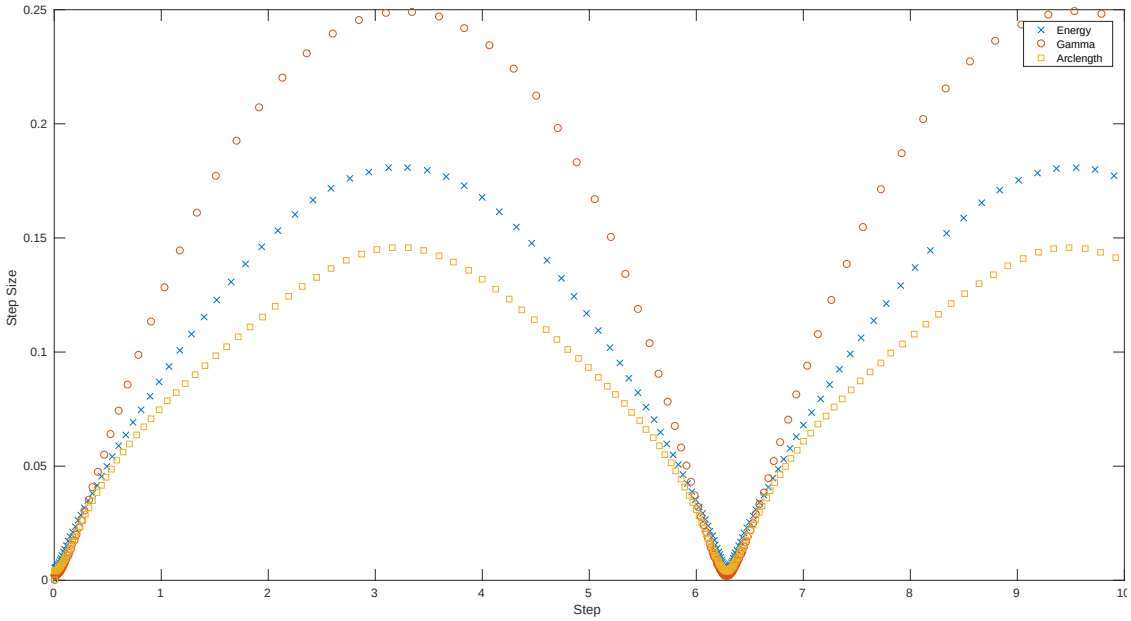

FIGURE 6. The time-steps taken for the various choices of monitor functions. Energy is the monitor function (20), gamma is the monitor function (18), and arc length is the monitor function (19). The energy monitor and gamma monitor function performed the best in terms of fewest steps, lowest computational cost and lowest global error. Notice that (20) did not take the largest steps nor the smallest steps.

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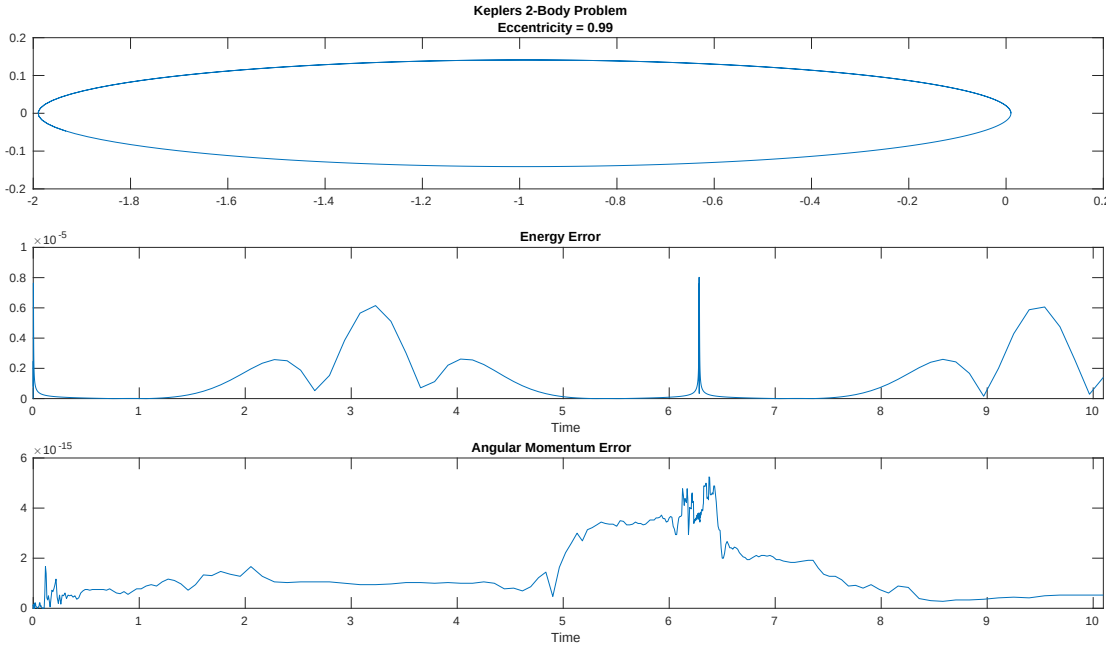

FIGURE 7. The monitor function (20) and HTVI4 applied to Kepler's 2-body planar problem with an eccentricity of 0.99. This choice of monitor function resulted in the fewest steps for an accuracy of 10^{-5} or better.