Variational Integrators for Almost-Integrable Systems

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Abstract We construct several variational integrators—integrators based on a discrete variational principle—for systems with Lagrangians of the form

\[ L = L_A + \varepsilon L_B, \]

with \( \varepsilon \ll 1 \), where \( L_A \) describes an integrable system. These integrators exploit that \( \varepsilon \ll 1 \) to increase their accuracy by constructing discrete Lagrangians based on the assumption that the integrator trajectory is close to that of the integrable system. Several of the integrators we present are equivalent to well-known symplectic integrators for the equivalent perturbed Hamiltonian systems, but their construction and error analysis is significantly simpler in the variational framework. One novel method we present, involving a weighted time-averaging of the perturbing terms, removes all errors from the integration at \( O(\varepsilon) \). This last method is implicit, and involves evaluating a potentially expensive time-integral, but for some systems and some error tolerances it can significantly outperform traditional simulation methods.

Keywords N-Body Problems · Hamiltonian Systems · Numerical Methods

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1 Introduction

Symplectic integrators have been used since their introduction in [Wisdom and Holman (1991)] for simulations of gravitational systems which are dominated by a central body. These integrators split the Hamiltonian for a system into two parts:

\[ H = H^{(A)} + \varepsilon H^{(B)}, \]  

where \( H^{(A)} \) represents the influence of the dominant central body on the bodies that orbit it, and \( \varepsilon H^{(B)} \), \( \varepsilon \ll 1 \), represents the mutual interactions of the bodies in orbit around it. (In our solar system, \( \varepsilon \sim 10^{-3} \); for stars in orbit around a central galactic black hole, \( \varepsilon \sim 10^{-6} \).) These integrators are a composition of evolutions under the separate pieces of the Hamiltonian, which are individually integrable. The integrators in [Wisdom and Holman (1991)] have a trajectory error which scales as \( O(\varepsilon h^3) \) over a single step of size \( h \). [McLachlan (1995)].
Chambers and Murison (2000), and Laskar and Robutel (2001) present improvements to the basic leapfrog scheme in Wisdom and Holman (1991) which involve more composition steps to eliminate error terms at $O(\varepsilon)$; these integrators have errors after a single step of size $h$ which scale as $O(\varepsilon^2 h^3) + O(\varepsilon h^{n+1})$ and are known as pseudo-high-order integrators. Wisdom et al. (1996) introduced correctors which can completely eliminate errors at $O(\varepsilon)$ from the integration.

In this work, we present integrators derived from a Lagrangian of the form

$$L = L^{(A)} + \varepsilon L^{(B)}$$

(2)

based on a discrete variational principle which incorporates the dominant $L^{(A)}$ motion of the system. These variational integrators subsume traditional symplectic integrators. Section 2 provides a brief introduction to variational integrators; Marsden and West (2001) provides a thorough mathematical grounding for these integrators and discusses in detail their properties. Lew et al. (2004) provides another introduction to the topic, and discusses the use of variational integrators in a space-time (PDE) context. Lee et al. (2007) demonstrate a geometrically exact method for simulating full-body dynamics in orbital mechanics with a variational integrator.

In this paper, we derive the pseudo-high-order integrators presented in McLachlan (1995), Chambers and Murison (2000), and Laskar and Robutel (2001) using the variational framework. The occurrence of the Gauss-Lobatto quadrature coefficients in the composition formulas for these integrators is a natural consequence in this framework of using Gauss-Lobatto quadrature to approximate the contribution of $L^{(B)}$ to the action integral. We exploit the flexibility of the variational framework to derive a novel implicit integrator which eliminates all errors from the trajectory at $O(\varepsilon)$ through averaging of the perturbing Lagrangian, $\varepsilon L^{(B)}$, along the trajectory of $L^{(A)}$. We present numerical evidence in Section 4 that this latter integrator can be more efficient than standard symplectic integrators for some systems of physical interest in spite of its higher cost per step. We argue in Section 3.2 that this method should be more stable at large stepsize for eccentric systems than the standard symplectic integrators, even with symplectic correctors.

In this work we use the notation of Sussman et al. (2001). The function which is the derivative of a function $f$ is denoted $Df$; if $f$ takes a vector argument $x$, then $Df(x)$ is a co-vector. Similarly, we denote the function which is the partial derivative with respect to the $i$th argument (counting from zero) of a function, $g$, of multiple arguments by $\partial_i g$. Some examples relating our notation to traditional notation:

$$Df(x) = \frac{df}{dx}(x) \text{ or } \frac{\partial f}{\partial x}(x)$$

(3)

$$\partial_i f(x, y, z) = \frac{\partial f(x, b, z)}{\partial b} \bigg|_{b=y} \quad \text{or} \quad \frac{\partial f(x, b, z)}{\partial b} \bigg|_{b=y}. \quad \text{(4)}$$

2 Variational Integrators

We can construct a variational integrator for a mechanical system with Lagrangian $L(q, v)$—here assumed to be time-independent for simplicity—by considering the action for the system over a small interval of time Farr and Bertschinger (2007; Lew et al. 2004):

$$S(h, q_0, q_1) = \int_0^h dt \, L(q(t), Dq(t)), \quad \text{(5)}$$
where \(q(t)\) is the physical trajectory of the system with \(q(0) = q_0\) and \(q(h) = q_1\). We choose a function, called the *discrete Lagrangian*, which approximates the action integral:

\[
L_D(h, q_0, q_1) \approx S(h, q_0, q_1).
\]

Then the *discrete Euler-Lagrange equations*

\[
\partial_1 L_D(h, q_0, q_1) = -p_0 \tag{7}
\]

\[
\partial_2 L_D(h, q_0, q_1) = p_1 \tag{8}
\]

define an integrator, \((q_0, p_0) \mapsto (q_1, p_1)\). Depending on the structure of \(L_D\), equation \((7)\) may be implicit for \(q_1\).

For example, consider the Harmonic oscillator, which has Lagrangian

\[
L = \frac{1}{2} (v^2 - q^2) \tag{9}
\]

in suitable units. Adopt the ansatz that \(q(t) = q_0 + (q_1 - q_0)(t - t_0)/h\); we can construct a discrete Lagrangian using the midpoint rule:

\[
L_D(h, q_0, q_1) = hL \left( \frac{q_0 + q_1}{2}, \frac{q_1 - q_0}{h} \right). \tag{10}
\]

The integrator equations \((7)\) and \((8)\) can be solved explicitly for \(q_1\) and \(p_1\). The result is

\[
q_1 = \frac{4 - h^2}{4 + h^2} q_0 + \frac{4h}{4 + h^2} p_0 \tag{11}
\]

\[
p_1 = -\frac{4h}{4 + h^2} q_0 + \frac{4 - h^2}{4 + h^2} p_0. \tag{12}
\]

Comparing with the actual solution

\[
q(t) = q_0 \cos(t) + p_0 \sin(t) \tag{13}
\]

\[
p(t) = -q_0 \sin(t) + p_0 \cos(t), \tag{14}
\]

we see that the integrator follows the exact trajectory but with phase error—that is, \(q_1 = q(h + \delta t)\) and \(p_1 = p(h + \delta t)\) for some phase error \(\delta t\).

One way to understand variational integrators is to recall that the action is an \(F_1\)-type generating function for the canonical transformation that implements time-evolution (see, e.g., [Sussman et al. (2001), pp. 415–416]). The action defines the \(F_1\)-type map, \((q, p) \mapsto (Q, P)\), via

\[
\partial_1 S(h, q, Q) = -p \tag{15}
\]

\[
\partial_2 S(h, q, Q) = P; \tag{16}
\]

these are just equations \((7)\) and \((8)\), with the discrete Lagrangian—an approximate action—replaced by the true action.

Alternately, consider our approximation to the action over a longer interval:

\[
S_{tot}(q_0, q_1, q_2, \ldots) = S(h, q_0, q_1) + S(h, q_1, q_2) + \ldots \\
\approx L_D(h, q_0, q_1) + L_D(h, q_1, q_2) + \ldots \tag{17}
\]
Then equations (7) and (8) express the stationarity of our approximation to the action with respect to the intermediate positions $q_1, q_2, \ldots$:

$$\partial_1 S_{\text{tot}} (q_0, q_1, q_2, \ldots) \approx \partial_2 L_D (h, q_0, q_1) + \partial_1 L_D (h, q_1, q_2) = p_1 - p_1 = 0. \quad (18)$$

Because the mapping in equations (7) and (8) is the extremization of an approximation to the action, it shares many of the desirable properties of the exact trajectory which extremizes the true action. For example, if $L_D$ has symmetries, a discrete Nöther’s theorem implies that the corresponding momenta are conserved. Also, the mapping is symplectic: denote the mapping by $F$. Then the symplectic form on phase space $dq \wedge dp$ is invariant under pushforward by $F$:

$$F^* (dq \wedge dp) = dq \wedge dp. \quad (19)$$

Finally, it is possible to show via backward error analysis (Lew et al. 2004) that the mapping implements the exact evolution for some Lagrangian $L$ which is close to $L$. Therefore, the evolution under $L_D$ remains on a constant-energy surface in phase space for $L$. Because $L$ is close to $L$, the evolution under $L_D$ always remains close to the constant-energy surface of $L$, so the long-term energy error of the mapping under $L_D$ is bounded.

The order of error in the mapping of equations (7) and (8) is the same as the order of error in the action approximation $L_D$ (Marsden and West 2001, Theorem 2.3.1). That is, if

$$L_D (h, q(0), q(h)) = S(h, q(0), q(h)) + O(h^{n+1}), \quad (20)$$

where $q(t)$ is a stationary-action trajectory, then the mapping defined by equations (7) and (8) approximates the physical trajectory to $O(h^{n+1})$, and therefore defines an $n$-th order integrator for $L$. We shall exploit this result in the error analysis of the integrators presented in this paper.

### 2.1 Multi-Point Variational Integrators

It is often advantageous to allow the discrete trajectory to pass through intermediate points between $q_0$ and $q_1$. For example, we may imagine that the discrete trajectory is a polynomial in time which interpolates between the positions $q_0, q'_0, q''_0, \ldots, q^n_0, q_1$. With intermediate positions, the discrete Euler-Lagrange equations become

$$\partial_1 L_D \left( h, q_0, q'_0, q''_0, \ldots, q^{(n)}_0, q_1 \right) = -p_0 \quad (21)$$

$$\partial_{i+1} L_D \left( h, q_0, q'_0, q''_0, \ldots, q^{(i)}_0, q_1 \right) = 0, \quad i = 1, 2, \ldots, n \quad (22)$$

$$\partial_{n+2} L_D \left( h, q_0, q'_0, q''_0, \ldots, q^{(n)}_0, q_1 \right) = p_1. \quad (23)$$

The intermediate equations express that the action is stationary with respect to the intermediate positions, while the other equations give the time-evolution canonical transformation.

We can always (in principle) re-express any multi-point discrete Lagrangian as an equivalent two-point discrete Lagrangian by solving the intermediate equations for the intermediate positions in terms of the start and end positions:

$$L_D (h, q_0, q_1) = L_D \left( h, q_0, q'_0 (h, q_0, q_1), \ldots, q^{(n)}_0 (h, q_0, q_1), q_1 \right), \quad (24)$$
where the functions \( q_0'(h, q_0, q_1), \ldots, q_n'(h, q_0, q_1) \) solve
\[
\partial_{t_1} L_D \left( h, q_0, q_0', q_0'', \ldots, q_0^{(n)}, q_1 \right) = 0, \quad i = 1, \ldots, n. \tag{25}
\]

Applying equations \( \ref{eq:26} \) and \( \ref{eq:27} \) to \( L_D \) gives the same trajectory as the discrete Euler-Lagrange equations for \( L_D \).

One way to form multi-point discrete Lagrangians is to chain together two separate discrete Lagrangians:
\[
L_D \left( h, q_0, q_0', q_1 \right) = L_D^{(1)} \left( h, q_0, q_0' \right) + L_D^{(2)} \left( h, q_0', q_1 \right). \tag{26}
\]

A quick calculation shows that the evolution under \( L_D \) is a composition of evolution under \( L_D^{(2)} \) with that under \( L_D^{(1)} \).

A common way to construct variational integrators of various orders is to assume that the trajectory of the system is a polynomial in time which passes through some discretization points: \( q = q \left( t; q_0, q_0', \ldots, q_0^{(n)}, q_1 \right) \). One then forms a discrete Lagrangian using a quadrature rule on the action integral evaluated on the discrete trajectory:
\[
L_D \left( h, q_0, q_0', \ldots, q_0^{(n)}, q_1 \right) = h \sum_i w_i L \left( q \left( t_i; q_0, q_0', \ldots, q_0^{(n)}, q_1 \right), \partial_t q \left( t_i; q_0, q_0', \ldots, q_0^{(n)}, q_1 \right) \right), \tag{27}
\]
where \( \{w_i, t_i\} \) are the weights and times of a quadrature rule. The order of the resulting map is determined by the orders of the polynomial interpolation and quadrature rule.

3 Almost-Integrable Systems

An almost-integrable system has a Lagrangian of the form
\[
L = L^{(A)} + \epsilon L^{(B)}, \tag{28}
\]
where \( \epsilon \ll 1 \), and the trajectories of \( L^{(A)} \) are calculable analytically (or at least efficiently). In contrast to the general Lagrangian, where little can be said about trajectories, we expect that the trajectories of \( L \) are going to be, in some sense, close to those of \( L^{(A)} \). We should take advantage of this fact when designing variational maps to approximate the trajectories of \( L \) instead of blindly assuming polynomial-in-time motion as discussed at the end of the last section.

The integrators we are about to describe all use as a component a particular discrete Lagrangian:
\[
L_D^{(A)} \left( h, q_A(0), q_A(h) \right) \equiv \int_0^h dt L^{(A)} \left( q_A(t), Dq_A(t) \right), \tag{29}
\]
where \( q_A(t) \) is the trajectory corresponding to the Lagrangian \( L^{(A)} \). \( L_D^{(A)} \) is the exact action for the A-subsystem on its trajectories; applying equations \( \ref{eq:28} \) and \( \ref{eq:29} \) to \( L_D^{(A)} \) gives the \( q_A \) trajectory:
\[
\partial_1 L_D^{(A)} \left( h, q_A(0), q_A(h) \right) = -p_A(0) \tag{30}
\]
\[
\partial_2 L_D^{(A)} \left( h, q_A(0), q_A(h) \right) = p_A(h). \tag{31}
\]
In general, it is not necessary to compute \( L_D^{(A)} \); all that is necessary is to be able to efficiently compute the mapping defined by equations \( \ref{eq:30} \) and \( \ref{eq:31} \).
3.1 Composition Maps Using Quadrature Rules

In this subsection we will show how some well-known symplectic maps are equivalent to variational integrators and we will analyze their errors in the variational framework. Both the derivation and error analysis are considerably simpler in the variational framework. We will assume that

\[ L^B(q,v) = -V^B(q); \]  

(32)

this common case is required for the integrators we discuss to be compositional.

We will see that the well-known symplectic integrators in McLachlan (1995), Chambers and Murison (2000), and Laskar and Robutel (2001) result from using Gauss-Lobatto quadrature to approximate

\[ -\int_0^h dt V^B(q(t)) \]  

(33)

in the discrete Lagrangian, assuming \( q_A \) trajectories between the quadrature points. In McLachlan (1995), Chambers and Murison (2000), and Laskar and Robutel (2001) the coefficients for these mapping integrators come from the solution to algebraic equations involving iterated commutators of the Hamiltonians \( H^A \) and \( H^B \), and turn out to be Gauss-Lobatto quadrature weights and times. In the framework of this paper, the Gauss-Lobatto quadrature coefficients arise naturally from the attempt to approximate the time-integral of \( V^B \) to a given order.

3.1.1 Kick-Drift-Kick Leapfrog

Suppose we choose

\[ L_D(h,q_0,q_1) = L_D^A(h,q_0,q_1) + \varepsilon L_D^B(h,q_0,q_1) \]

\[ = L_D^A(h,q_0,q_1) - \varepsilon \frac{h}{2} \left[ V^B(q_0) + V^B(q_1) \right]. \]  

(34)

Here we have simply used the trapezoidal rule (a two-point Gauss-Lobatto quadrature)

\[ \int_a^b dx f(x) \approx \frac{b-a}{2} [f(a) + f(b)] \]  

(35)

to approximate the contribution to the action from \( L_B \). Applying equations (7) and (8) to this discrete Lagrangian, we have

\[ -p_0 = \partial_1 L_D^A(h,q_0,q_1) - \varepsilon \frac{h}{2} DV^B(q_0) \]  

(36)

\[ p_1 = \partial_2 L_D^A(h,q_0,q_1) - \varepsilon \frac{h}{2} DV^B(q_1). \]  

(37)

These can be re-written in a suggestive way:

\[ \left( -p_0 - \varepsilon \frac{h}{2} DV^B(q_0) \right) = \partial_1 L_D^A(h,q_0,q_1) \]  

(38)

\[ p_1 = \partial_2 L_D^A(h,q_0,q_1) - \varepsilon \frac{h}{2} DV^B(q_1). \]  

(39)

The solution to the first equation is the \( q_1 \) that results from evolving \( \left( q_0, p_0 - \varepsilon h/2 DV^B(q_0) \right) \) forward by \( L^A \). The final momentum is then \( p_A = -\varepsilon \frac{h}{2} DV^B(q_1) \). In other words, we kick
by \(-\varepsilon \frac{h}{2}DV^{(B)}(q_0)\), drift by \(L^{(A)}\), and then kick by \(-\varepsilon \frac{h}{2}DV^{(B)}(q_1)\). The algorithm is kick-drift-kick leapfrog—see, e.g. [Wisdom and Holman (1991)].

Using the variational framework to analyze the error of kick-drift-kick leapfrog, we consider

\[
\Delta \equiv L_D(h, q(0), q(h)) - S(h, q(0), q(h)).
\]  

(40)

The trajectory error of kick-drift-kick leapfrog will be of the same order as \(\Delta\). Expanding, we have

\[
\Delta = \Delta_A + \varepsilon \Delta_B
\]

\[
= \int_0^h dt \left[ L_A(q_A(t; q(0), q(h)), Dq_A(t; q(0), q(h))) - L_A(q(t), Dq(t)) \right]
\]

\[
- \varepsilon \left[ \frac{h}{2} \left( V^{(B)}(q(0)) + V^{(B)}(q(h)) \right) - \int_0^h dt V^{(B)}(q(t)) \right].
\]  

(41)

For the first term, we have

\[
\Delta_A = \frac{\delta}{\delta q_A} \left[ \int_0^h dt L_A(q_A(t; q(0), q(h)), Dq_A(t; q(0), q(h))) \right] \delta q_A
\]

\[
+ \frac{\delta^2}{\delta q_A^2} \left[ \int_0^h dt L_A(q_A(t; q(0), q(h)), Dq_A(t; q(0), q(h))) \right] \delta q_A^2 + O(\delta q_A^3),
\]  

(42)

where \(\delta q_A\) is the trajectory difference between \(q_A\) and \(q\). \(\delta q_A\) is \(O(\varepsilon h)\) because the Lagrangian depends on the velocity, and the two trajectories must differ at first order in \(h\) in their velocities (since they feel different forces at order \(\varepsilon\)). But, the trajectory \(q_A\) is the solution to the Euler-Lagrange equations for \(L_A\), so the first order variation of \(L_A\) vanishes on \(q_A\), and only the second-order term contributes. Therefore, we have

\[
\Delta_A = O(\varepsilon^2 h^3).
\]  

(43)

For the second term of equation (41), we have

\[
\varepsilon \Delta_B = \varepsilon \left[ \delta \left( \frac{h^3}{3} \right) \right] = O(\varepsilon h^3),
\]  

(44)

arising from the truncation error in the quadrature rule. Putting the two terms together, we see that

\[
\Delta = \Delta_A + \varepsilon \Delta_B = O(\varepsilon h^3) + O(\varepsilon^2 h^3),
\]  

(45)

with the term at \(O(\varepsilon)\) arising from the quadrature rule error, and the term at \(O(\varepsilon^2)\) arising from the error in \(L^{(A)}_D\). This will be a general feature of the integrators in this section: the quadrature error determines the \(O(\varepsilon)\) integrator error, while the \(O(\varepsilon^2)\) error is determined by the error in the \(L^{(A)}_D\) term.
3.1.2 S4B

Consider choosing a higher-order quadrature rule for the $\epsilon L^{(B)}$ term. For example, a three-point Gauss-Lobatto quadrature rule, with $q_A$ trajectories between the quadrature points:

$$L_D (h, q_0, q'_0, q_1) = L_D^{(A)} \left( \frac{h}{2}, q_0, q'_0 \right) + L_D^{(A)} \left( \frac{h}{2}, q'_0, q_1 \right) - \epsilon \frac{h}{6} \left[ V^{(B)} (q_0) + 4V^{(B)} (q'_0) + V^{(B)} (q_1) \right]$$

(46)

As above, this integrator can be written as a sequence of kicks and drifts: a kick by $-\epsilon \frac{h}{2} DV (q_0)$, a drift by $h/2$ with respect to $L^{(A)}$ to $q'_0$, a kick by $-\epsilon \frac{2h}{3} DV (q'_0)$, a drift by $h/2$ with respect to $L^{(A)}$ to $q_1$, and a final kick by $-\epsilon \frac{h}{2} DV (q_1)$.

As before the error introduced by the $L_D^{(A)}$ part is second order in $\delta q_A$, or $O(\epsilon^2 h^3)$, while the quadrature rule introduces an error in the $V^{(B)}$ part of $O(\epsilon L^3)$. (There is an additional error in the quadrature arising from the trajectory error $\delta q_A$, which contributes at $O(\epsilon^2 h^3)$ because the potential is independent of the velocity difference between $q$ and $q_A$.)

Thus, the error in this method scales as

$$\Delta = O \left( \epsilon h^3 \right) + O(\epsilon^2 h^3).$$

(47)

It belongs to a class of integrators known as “pseudo-high-order”, first discovered by McLachlan (1995), and introduced to the astronomical community in Chambers and Murison (2000) and Laskar and Robutel (2001). These integrators are useful because, for small enough $\epsilon$, they behave as high-order integrators, even though they are formally second order. The name of this section (and the integrator) is S4B, from Chambers and Murison (2000).

McLachlan (1995) originally derived the coefficients of the kicks and kicks for this integrator by attempting to eliminate commutator terms in the Lie series for Hamiltonian evolution; he noted that the coefficients which eliminate the desired first-order-in-$\epsilon$ terms are identical to the Gauss-Lobatto quadrature coefficients. In this work, we can understand this as a consequence of attempting high-order quadrature of the contribution of $L^{(B)}$ to the action.

3.1.3 S6B

Consider now the sixth-order Gauss-Lobatto quadrature for the $L^{(B)}$ terms, interspersed with $q_A$ evolution:

$$L_D (h, q_0, q'_0, q''_0, q_1) =$$

$$L_D^{(A)} \left( \frac{h (5 - \sqrt{5})}{10}, q_0, q'_0, q''_0 \right) + L_D^{(A)} \left( \frac{h}{\sqrt{5}}, q'_0, q''_0 \right) + L_D^{(A)} \left( \frac{h (5 - \sqrt{5})}{10}, q''_0, q_1 \right)$$

$$- \epsilon \frac{h}{12} \left[ V^{(B)} (q_0) + 5V^{(B)} (q'_0) + 5V^{(B)} (q''_0) + V^{(B)} (q_1) \right]$$

(48)

This is exactly the sequence of drifts and kicks for the S6B integrator (Chambers and Murison 2000). Once again, the error is a combination of errors from the quadrature at $O(\epsilon)$, and errors from $L_D^{(A)}$ at $O(\epsilon^2)$:

$$\Delta = O \left( \epsilon h^3 \right) + O(\epsilon^2 h^3)$$

(49)
3.2 An $O(\varepsilon^2)$ Method

We can eliminate all errors at $O(\varepsilon)$ by using for $L_D^{(B)}$ the exact integral of $V^{(B)}$ along the $q_A$ trajectory. Define

$$L_D(h, q_0, q_1) = L_D^{(A)}(h, q_0, q_1) + \varepsilon L_D^{(B)}(h, q_0, q_1) = L_D^{(A)}(h, q_0, q_1) - \varepsilon \int_0^h dt \int (q_A(t; q_0, q_1)).$$

(50)

Applying equation (7) to $L_D$, and moving the $L_D^{(B)}$ term to the left-hand-side, we obtain

$$- \left( p_0 + \varepsilon \partial_1 L_D^{(B)}(h, q_0, q_1) \right) = L_D^{(A)}(h, q_0, q_1),$$

(51)

which we must solve for $q_1$. The momentum kick,

$$\varepsilon \partial_1 L_D^{(B)}(h, q_0, q_1) = -\varepsilon \int_0^h dt \int (q_A(t; q_0, q_1)) \partial_1 q_A(t; q_0, q_1),$$

(52)

is the time-averaged force along an $L^{(A)}$ trajectory weighted by $\partial_1 q_A(t; q_0, q_1)$—in general, this weight favors the initial periods of the trajectory, since $q_A(h; q_0, q_1) = q_1$ independent of $q_0$. Once the point $q_1$ is determined, the new momentum is

$$p_1 = \partial_2 L_D(h, q_0, q_1) = p_1^{(A)} + \varepsilon \partial_2 L_D^{(B)}(h, q_0, q_1).$$

(53)

Here, the kick

$$\varepsilon \partial_2 L_D^{(B)}(h, q_0, q_1) = -\varepsilon \int_0^h dt \int (q_A(t; q_0, q_1)) \partial_2 q_A(t; q_0, q_1),$$

(54)

is the time-averaged force along an $L^{(A)}$ trajectory weighted by $\partial_2 q_A(t; q_0, q_1)$—which tends to favor later points in the trajectory, since $q_A(0; q_0, q_1) = q_0$ independent of $q_1$. Because the momentum kicks are related to the time-averaged force along the integrator trajectory, the integrator has a flavor of averaging. Timesteps with this integrator can be as large as the time it takes the trajectory to deviate on average from $q_A$, in contrast to the integrators from the previous subsection. In those integrators timesteps must be small enough that both $q_A$ adequately approximates the trajectory and that the sequence of kicks adequately approximates the averaged force. Evaluating the averaged force in the way that the $O(\varepsilon^2)$ variational method does removes this second restriction. This could be important in the simulation of highly eccentric systems.

3.2.1 Error Analysis

The error from the $V^{(B)}$ integral is

$$\varepsilon \Delta B = \varepsilon \frac{\delta}{\delta q_A} \left[ \int_0^h dt \int (q_A(t; q_0, q_1)) \right] \delta q_A + \mathcal{O}(\varepsilon^2 h^3).$$

(55)

Because $V^{(B)}$ depends only on $q$ and not on $\dot{q}$, $\delta q_A$ scales as $\mathcal{O}(\varepsilon h^2)$ (the true trajectory $q$ and $q_A$ must differ at order $\varepsilon h^2$ because they feel different forces of size $\varepsilon$).
Combining the error in equation (55) with $\Delta$, we obtain

$$\Delta = \mathcal{O}(\epsilon^2 h^3),$$

resulting in a method which is formally second-order, but has no errors at $\mathcal{O}(\epsilon)$.

The method is implicit; one must solve equation (7),

$$- p_0 = \partial_1 L_D(h, q_0, q_1),$$

for $q_1$. This can be accomplished through Newton iteration, or through the iterative method which follows. (In practice, for small $\epsilon < 10^{-3}$ and systems of modest dimension, we find that the iterative method is more efficient than Newton iteration.) Define the sequence $\{q_1^{(i)}\}$ by

$$- (p_0 - \epsilon \partial_1 L_D^B(h, q_0, q_1^{(i-1)})) = \partial_1 L_D^A(h, q_0, q_1^{(i)}).$$

If $q_1^{(i-1)}$ is known, then $q_1^{(i)}$ is just the evolution of the state $(q_0, p_0 - \epsilon \partial_1 L_D^B(h, q_0, q_1^{(i-1)}))$ by $L_A$. For small $\epsilon$, this sequence $\{q_1^{(i)}\}$ converges linearly to the desired $q_1$.

The efficiency of this method will depend on how tractable it is to evaluate

$$\int_0^h dt V^B(q_A(t; q_0, q_1))$$

as a function of the endpoints $q_0$ and $q_1$. In the next section, we will examine the performance of the methods introduced in this section on some example problems.

4 Example Calculations

In this section, we apply the integrators from the previous section to some example problems.

4.1 The Perturbed SHO

Consider the Lagrangian

$$L(q, v) = \frac{1}{2} (v^2 - q^2) - \frac{\epsilon}{3} q^3.$$

This represents a simple harmonic oscillator (with natural period $2\pi$) with an additional force $F(q) = -\epsilon q^2$. For $\epsilon \ll 1$, the system is amenable to solution using the methods from the previous section. In particular, because the perturbation term is a polynomial in $q$, we can easily compute the $\mathcal{O}(\epsilon^2)$ discrete Lagrangian:

$$L_D(h, q_0, q_1) = \int_0^h dt L(q_A(t; q_0, q_1), Dq_A(t; q_0, q_1)) =$$

$$\frac{1}{2} (q_0^2 + q_1^2) \cot(h) - q_0 q_1 \csc(h)$$

$$- \epsilon \left[ (q_0 + q_1) (2q_0^2 + q_0 q_1 + 2q_1^2) + (q_0^3 + q_1^3) \cos(h) \right] \sec^2 \left( \frac{h}{2} \right) \tan \left( \frac{h}{2} \right).$$

Figure 1 displays the maximum energy error over a simulation of the oscillator with a total time $T = 1000$ as a function of the timestep $h$ for the various methods in Section 3. We can see in Figure 1 that the $\mathcal{O}(\epsilon^2)$ variational method significantly outperforms the other methods at large timesteps.
4.2 Jupiter, Saturn, and the Sun

This subsection reports on simulations of the Jupiter-Saturn-Sun system with realistic initial conditions. The Lagrangian for this system is

\[
L = \frac{1}{2} \left( m_\odot v_\odot^2 + m_J v_J^2 + m_S v_S^2 \right) + \frac{Gm_\odot m_J}{r_{\odot J}} + \frac{Gm_\odot m_S}{r_{\odot S}} + \frac{Gm_J m_S}{r_{JS}}. \tag{62}
\]

The well-known Jacobi transformation (see, e.g. \cite{WisdomHolman91}) can transform this Lagrangian into a sum of center-of-mass motion, two Kepler Lagrangians, and perturbing terms with magnitude \( \mathcal{O}(\varepsilon^2) \sim m_J/m_\odot \sim 10^{-3} \).

In this paper, we evaluate the time-average of the perturbing terms—which are essentially the disturbing function for the three-body problem—for the \( \mathcal{O}(\varepsilon^2) \) variational integrator on the \( q_A \) (Kepler) trajectory using numerical quadrature. Numerical quadrature is adaptive; each quadrature point corresponds to a (weighted) kick at that time, and quadrature points are allocated non-uniformly on the interval \([0,h]\) to best approximate the integral. With this technique, we can use the \( \mathcal{O}(\varepsilon^2) \) variational method on highly elliptical orbits with a large timestep without loss of accuracy, since the quadrature routine will allocate points densely near pericenter. The other integration methods, which allocate quadrature points at fixed fractions of the stepsize, must be run with a small enough stepsize to resolve rapidly changing forces near pericenter passage throughout the entire orbit.

Figure 2 displays the energy error in a simulation of the Jupiter-Saturn-Sun system for approximately 20 Jupiter orbits (which corresponds to approximately 240 years) versus timestep. For a maximum tolerable error of \( \varepsilon^2 \sim 10^{-6} \), the \( \mathcal{O}(\varepsilon^2) \) variational integrator can take stepsizes of order 10 orbits, while the other methods do not perform well until there are several kicks per orbit. However, for high-accuracy integrations the errors in the
methods (excepting KDK) are comparable, and the extra cost of the averaging in the $O(\varepsilon^2)$ variational integrator when compared to the other methods makes it sub-optimal.

4.3 Small-mass Jupiter, Saturn, and the Sun

This subsection reports on a simulation with the same initial conditions as Section 4.2, but with the masses of Jupiter and Saturn reduced by a factor of $10^{-3}$. This brings $\varepsilon \sim 10^{-6}$, roughly in line with the size of the perturbing interaction one might find in a cluster of stars around a super-massive black hole in the center of a galaxy.

Figure 3 presents the relative energy error versus timestep for a simulation of this smaller-$\varepsilon$ system over approximately 100 Jupiter orbits. In this circumstance, the $O(\varepsilon^2)$ variational integrator significantly outperforms the other integrators, even for the (relatively severe) error budget of $10^{-12}$. It can take steps which are approximately $10^3$ longer than those of the other integrators at the same energy error budget, more than compensating for the expensive time-averaging and implicit nature of the algorithm.

In Figure 4 we plot the trajectory error of the various methods at the end of the simulation period (100 Jupiter orbits). The $O(\varepsilon^2)$ variational method outperforms the other methods by approximately a factor of $10^3$ in stepsize at a relative trajectory error of $10^{-10}$.
Fig. 3 Maximum relative energy error in a simulation analogous to the one in Section 4.2 except with Jupiter and Saturn’s masses reduced by a factor of $10^{-3}$ (note that Jupiter still has a 12-year period). The curves are for the following algorithms: KDK (plus), S4B (circles), S6B (stars), and $O(\varepsilon^2)$ variational (dots). In this system $\varepsilon \sim 10^{-6}$, and we see that the $O(\varepsilon^2)$ variational integrator can take stepsizes which are $\sim 10^3$ larger than other algorithms for an error budget of $10^{-12}$.

Fig. 4 Relative phase-space (trajectory) error at the end of a simulation analogous to the one in Section 4.2 except with Jupiter and Saturn’s masses reduced by a factor of $10^{-3}$ (note that Jupiter still has a 12-year period). The curves are for the following algorithms: KDK (plus), S4B (circles), S6B (stars), and $O(\varepsilon^2)$ variational (dots). In this system $\varepsilon \sim 10^{-6}$, and we see that the $O(\varepsilon^2)$ variational integrator can take stepsizes which are $\sim 10^3$ larger than other algorithms for a phase-space error budget of $10^{-10}$. 
5 Conclusion

The variational framework subsumes standard symplectic methods. In this work, we have presented the pseudo-high-order integrators of McLachlan (1995), Chambers and Murison (2000), and Laskar and Robutel (2001) from the variational viewpoint for systems with Lagrangian \( L = L^A + \epsilon L^B \). In addition, we have used the variational framework to derive a novel implicit integrator which uses the average perturbing Lagrangian over trajectories of the dominant Lagrangian to remove all errors from the integration at \( \mathcal{O}(\epsilon) \). We have presented numerical evidence that, for small \( \epsilon \), this latter integrator is more efficient than standard pseudo-high-order symplectic integrators for perturbed systems. It would be interesting to investigate the performance of this latter integrator with various analytical approximations to the average of the perturbing Lagrangian.

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