"SLIPLECTIC" INTEGRATORS: VARIATIONAL INTEGRATORS FOR GENERAL NONCONSERVATIVE SYSTEMS

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ABSTRACT

Symplectic integrators are widely used for long-term integration of conservative astrophysical problems due to their ability to preserve the constants of motion; however, they cannot in general be applied in the presence of nonconservative interactions. In this Letter, we develop the “slimplectic” integrator, a new type of numerical integrator that shares many of the benefits of traditional symplectic integrators yet is applicable to general nonconservative systems. We utilize a fixed-time-step variational integrator formalism applied to the principle of stationary nonconservative action developed in Galley et al. As a result, the generalized momenta and energy (Noether current) evolutions are well-tracked. We discuss several example systems, including damped harmonic oscillators, Poynting–Robertson drag, and gravitational radiation reaction, by utilizing our new publicly available code to demonstrate the slimplectic integrator algorithm. Slimplectic integrators are well-suited for integrations of systems where nonconservative effects play an important role in the long-term dynamical evolution. As such they are particularly appropriate for cosmological or celestial N-body dynamics problems where nonconservative interactions, e.g., gas interactions or dissipative tides, can play an important role.

Key words: celestial mechanics – methods: numerical – planets and satellites: dynamical evolution and stability

1. INTRODUCTION

Symplectic integrators are a class of mappings that allow for numerical integration of conservative dynamical systems and which, up to round-off, exactly preserve certain constants of motion (e.g., the symplectic form). As a result the integrations do not suffer from numerical “dissipation” which would cause an unphysical drift over many dynamical times. Due to these properties, symplectic integrators are widely used in the long-term integration of many physical systems, particularly in celestial dynamics (Glädman et al. 1991; Wisdom & Holman 1991; Levison & Duncan 1994; Reis & Tamayo 2015).

Conservative variational integrators (see, e.g., Marsden & West 2001) are a subclass of symplectic integrators where the mappings are determined by the extremization of a discretized action. The discretized action can inherit the symmetries of the full action such that, by Noether’s theorem, the discrete equations of motion exactly conserve the symplectic form and the momenta. Since discretizing the time coordinate breaks the continuous time-shift symmetry, fixed-time-step variational integrators that preserve the symplectic form and the momenta cannot also conserve energy (Ge & Marsden 1988). However, the energy error tends to be bounded by a constant, even over long integration times (see, e.g., Lew et al. 2004 and references therein), in contrast with traditional integration methods where the error tends to grow with time.

Variational integrators can be applied to some dissipative problems using the Lagrange–d’Alembert approach (Marsden & West 2001; Lew et al. 2004). Here, we utilize the more general nonconservative action principle, recently developed by Galley (2013) and Galley et al. (2014). This formalism was developed to accommodate generically the causal dynamics of untracked or inaccessible degrees of freedom that might result from an integrating-out or coarse-graining procedure at the level of an action/Lagrangian/Hamiltonian.

In this Letter, we develop variational integrators from the nonconservative action principle. The resulting mappings are no longer symplectic, as the symplectic form (and momenta) are no longer conserved, but evolve according to the nonconservative dynamics. We instead refer to this type of numerical integrator as “slimplectic” since phase space volumes tend to slim down for dissipative systems. We show that our method inherits many of the same performance features of the symplectic integrator. Previous works have demonstrated some success by including weakly dissipative forces in second-order symplectic integrators (see, e.g., Malhotra 1994; Cordeiro et al. 1996; Mikkola 1997; Hamilton et al. 1999; Zhang & Hamilton 2007); in fact, these can be shown to be particular cases of our more general (arbitrary order) method. For brevity, we focus on a basic fixed-time-step slimplectic integrator leaving further developments, such as adaptive time-stepping and detailed discussion of Noether current evolution, to a longer follow-up paper.

2. NONCONSERVATIVE LAGRANGIAN MECHANICS

Nonconservative Lagrangian mechanics accommodates nonconservative interactions and effects by first formally doubling the degrees of freedom, \( q \rightarrow (q_1, q_2) \). The action describing the dynamics of these doubled variables is

\[
S = \int \Lambda(q_{1,2}, \dot{q}_{1,2}, t) dt
\]

(1)

where the (nonconservative) Lagrangian is

\[
\Lambda(q_{1,2}, \dot{q}_{1,2}, t) = L(q_1, \dot{q}_1, t) - L(q_2, \dot{q}_2, t) + K(q_{1,2}, \dot{q}_{1,2}, t)
\]

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3 Most symplectic integrators can be written as (local) variational integrators.

\[
\Lambda(q_{1,2}, \dot{q}_{1,2}, t) = L(q_1, \dot{q}_1, t) - L(q_2, \dot{q}_2, t)
\]
\( \Lambda \) is the usual Lagrangian, which is an arbitrary function of coordinates, velocity, and time and describes the conservative sector of the system (i.e., dynamics in the absence of nonconservative effects). However, \( K \) is another arbitrary function that couples the variables together, vanishes when \( q_1 = q_2 \), and accounts for any generic nonconservative interaction. Note that \( \Lambda \) is completely specified once \( L \) and \( K \) are given.

After all variations of \( S \) are performed the two variables are identified with each other, \( q_1 = q_2 = q \), which is called the physical limit (PL). In some cases, it is convenient to work with more physically motivated coordinates, \( q_1 = q_1 - q_2 \) and \( q_2 = (q_1 + q_2)/2 \). The former can often be considered like a virtual displacement and vanishes in the PL while the latter is the surviving physically relevant combination.

Requiring \( S \) to be stationary under variations of the doubled variables and taking the PL leads to nonconservative Euler–Lagrange equations of motion,

\[
\left[ \frac{d}{dt} \frac{\partial \Lambda}{\partial \dot{q}_r} - \frac{\partial \Lambda}{\partial q_r} \right]_{PL} = 0
\]

or in terms of \( L \) and \( K \),

\[
\left[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_r} - \frac{\partial L}{\partial q_r} \right]_{PL} = \left[ \frac{\partial K}{\partial \dot{q}_r} - \frac{d}{dt} \frac{\partial K}{\partial \dot{q}_r} \right]_{PL}.
\]

There are multiple ways to specify \( K \), which depend on the particular problem in question. More details about this aspect and the nonconservative action formalism in general can be found in Section 2 of Galley et al. (2014), including the evolution of Noether currents according to nonconservative processes described by \( K \).

3. VARIATIONAL INTEGRATORS FOR NONCONSERVATIVE SYSTEMS

Variational integrators numerically approximate the behavior of a system by implementing the exact equations of motion for a closely related discrete action (Marsden & West 2001; Brown 2006). Here we will apply it to the nonconservative action principle described above.

To construct a variational integrator we need to make a choice of discretization of the action integral

\[
S = \int_{t_0}^{t_f} \Lambda(q_{\pm}, \dot{q}_{\pm}, t) dt.
\]

A choice that provides a time-reversal symmetric discretization (thus an even order method; Farr & Bertschinger 2007) is Gauss–Lobatto quadrature, illustrated in Figure 1. On the time interval \( t \in [t_n, t_{n+1}] \) with \( \Delta t = t_{n+1} - t_n \), we have the set of \( r + 2 \) quadrature points \( t_n \), \( (t_n^{(i)})_{i=1}^{r+1}, t_{n+1}, \) with

\[
t_n^{(i)} \equiv t_n + (1 + x_i)\frac{\Delta t}{2},
\]

where \( x_0 = -1, x_{r+1} = +1, \) and \( x_i (i \in \{1 \ldots r\}) \) is the \( i \)th root of \( dP_{r+1}/dx \), the derivative of the \( (r+1) \)th Legendre polynomial, \( P_{r+1}(x) \). For a given nonconservative Lagrangian functional \( \Lambda(q_{\pm}, \dot{q}_{\pm}, t) \), we can approximate the degrees of freedom \( q_{n,\pm}(t) \equiv \phi_{n,\pm}(t) + \mathcal{O}(\Delta t^{r+3}) \) using the cardinal-function interpolation for this choice of quadrature points.

We then have the approximation \( \dot{q}_{n,\pm}(t) \approx \dot{\phi}_{n,\pm}(t) \), which can be conveniently evaluated at the quadrature points using the derivative matrix (see, e.g., Boyd 2001, 2015),

\[
D_{ij} = \left\{ \begin{array}{ll}
-(r+1)(r+2)/(2\Delta t) & i = j = 0 \\
(r+1)(r+2)/(2\Delta t) & i = j = r+1 \\
0 & i = j \neq 0, r+1 \end{array} \right.
\]

such that

\[
\dot{\phi}_{n,\pm}(t_n^{(i)}) = \sum_{j=0}^{r+1} D_{ij} q_{n,\pm}^{(j)} \equiv \dot{\phi}_{n,\pm}^{(i)}
\]

where for notational compactness we define \( t_n^{(0)} \equiv t_n \), \( t_n^{(r+1)} \equiv t_{n+1} \), and \( q_{n,\pm}^{(i)} \equiv q_{n,\pm}(t_n^{(i)}) \).

Using Gauss–Lobatto quadrature, any integral functional \( \int F dt \) (for example, \( F \in \{\Lambda, L, K\} \)) has a discrete-quadrature approximation on the time interval \([t_n, t_{n+1}] \). This discrete functional \( F_d \) is

\[
F_d \left( q_{n,\pm}, \{ q_{n,\pm}^{(i)} \}_{i=1}^{r+1}, q_{n+1,\pm}, t_n \right) \equiv \sum_{i=0}^{r+1} w_i F \left( q_{n,\pm}^{(i)}, \dot{q}_{n,\pm}^{(i)}, t_n^{(i)} \right) = F_d^n,
\]

where the Gauss–Lobatto quadrature weights \( w_i \) are given by

\[
w_i \equiv \frac{\Delta t}{(r+1)(r+2)|P_{r+1}(x_i)|^2}.
\]

Now we approximate the action over an interval \([t_0, t_{N+1}] \),

\[
S[t_0, t_{N+1}] = \int_{t_0}^{t_{N+1}} \Lambda(q_{\pm}, \dot{q}_{\pm}, t) dt \equiv S_d[t_0, t_{N+1}] + \mathcal{O}(\Delta t^{2r+3}) = S_d[t_0, t_{N+1}] + \mathcal{O}(\Delta t^{2r+3}).
\]
errors are comparable at each order, the RK energy errors grow roughly linearly
solution at each time. We see that while initially the RK and slimplectic energy
the energy evolution is accurately followed, though a phase shift is evident.
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sif}
Figure 2. Top: numerical solutions for the damped harmonic oscillator,
described by \( L = mq^2/2 - kq^2/2 \), \( K = -\lambda q \), with \( \lambda = 10^{-4} (m/\text{K})^{1/2} \), and
fixed time steps \( \Delta t = 0.1 (m/\text{K})^{1/2} \). Initial conditions were taken to be
\( q(0) = 1 \) and \( q(0) = 0 \). The second-order RK solution, shown in green,
is unstable for these parameters and diverges significantly. The fourth-order RK
solution (blue-dashed) cannot be readily distinguished from the fourth-order
slimplectic solution (solid-orange) in this plot. The second-order slimplectic
solution (solid-red) gives nearly the correct amplitude after \( \sim 10^6 \) time steps, as
the energy evolution is accurately followed, though a phase shift is evident.
Bottom: the fractional energy error relative to the energy given by the analytic
solution at each time. We see that while initially the RK and slimplectic energy
errors are comparable at each order, the RK energy errors grow roughly linearly
with time, while the slimplectic energy error remains bounded.

where the discretized action is defined as

\[
S_d(t_0, t_{N+1}) = \sum_{n=0}^{N} L_d\left(q_{n+1/2}, q_{n-1/2}, t_n\right) \approx \sum_{n=0}^{N} \left( \frac{\partial L_d}{\partial q_{n+1/2}} - \frac{\partial L_d}{\partial q_{n-1/2}} \right) \Delta t.
\]

We refer to this discretization choice as the Galerkin–Gauss–
Lobatto (GGL) method (Farr & Bertscherger 2007).

The discrete action \( S_d(t_0, t_{N+1}) \) from (10) can then be extremized over values \( q_{n-1} \) and \( q^{(i)}_{n} \) and the PL imposed, to
generate the discretized equations of motion for each \( n \in [1, N] \),

\[
\left[ \frac{\partial L_d}{\partial q_{n+1/2}} - \frac{\partial L_d}{\partial q_{n-1/2}} \right]_{\text{PL}} = 0,
\]

\[
\left[ \frac{\partial L_d}{\partial q_{n+1/2}} - \frac{\partial L_d}{\partial q_{n-1/2}} \right]_{\text{PL}} = 0,
\]

since from Figure 1, we see that each \( q^{(i)}_n \) only contributes to a
single \( \Lambda_d^{(i)} \) in the discretized action (10), while each \( q_{n-1} \) appears
in both \( \Lambda_d^{(i-1)} \) and \( \Lambda_d^{(i)} \).

In terms of \( L_d \) and \( K_d \), the equations of motion are

\[
\frac{\partial L_d}{\partial q_n} + \frac{\partial L_d}{\partial q_{n+1/2}} + \frac{\partial K_d}{\partial q_{n-1/2}} + \frac{\partial K_d}{\partial q_{n+1/2}} \right\}_{\text{PL}} = 0.
\]

We now introduce the discrete momenta \( p_n \), defining the
nonconservative (slimplectic) GGL variational integrator map
\( (q_n, p_n) \to (q_{n+1}, p_{n+1}) \), by splitting the equation of motion
(12a) so that Equations (12a) and (12b) become

\[
\frac{\partial L_d}{\partial q_n} + \frac{\partial L_d}{\partial q_{n+1/2}} + \frac{\partial K_d}{\partial q_{n-1/2}} + \frac{\partial K_d}{\partial q_{n+1/2}} \right\}_{\text{PL}} = 0.
\]

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\[
\frac{\partial L_d}{\partial q_n} + \frac{\partial L_d}{\partial q_{n+1/2}} + \frac{\partial K_d}{\partial q_{n-1/2}} + \frac{\partial K_d}{\partial q_{n+1/2}} \right\}_{\text{PL}} = 0.
\]

Given initial values of \( (q_n, p_n) \), the values of \( q_{n+1} \) are determined implicitly by (13a), while the values for the \( q^{(i)}_n \)
intermediate points are given implicitly by Equation (13c) for
\( i \in \{1 \ldots r\} \). The final momenta \( p_{n+1} \) can then be determined explicitly from (13b).

Noether’s theorem for conservative actions can be shown to
generalize to nonconservative systems where the correspond-
ing Noether currents evolve in time due to a non-zero
\( K \) (Galley et al. 2014). One can show that for continuous
symmetries of the conservative action, which remain after
 discretization, discrete Noether currents will also evolve due to
\( K \). Thus, translational or rotational symmetries, for
example, will generate discrete momenta that evolve according
to \( K \), up to round off and bias error (Brouwer 1937; 
Rein & Spiegel 2015). Additional error compared to the
physical evolution is only due to the discretization of the action.

The GGL discretization does not preserve the time-shift
symmetry preventing energy evolution from being precisely
tracked. However, the fractional energy error tends to
be oscillatory and bounded by a resolution and order-dependent
constant. We will defer more detailed discussion of Noether
current evolution to a longer follow-up paper in the interests
of space.

The resulting slimplectic maps are accurate up to
order \( 2r + 2 \). For \( r = 0 \), where no intermediate steps are
used, the quadrature method is the trapezoid rule, and the
variational integrator is second-order and equivalent to the
Störmer–Verlet “leap-frog“ integrator (Wendlandt &
Marsden 1997).

It is well known that second-order “leap-frog“ integrators
are used for dissipative systems, by inserting a dissipative
“kick“ force into the “kick-drift-kick“ ansatz, resulting in good
energy and momentum evolution properties. Our approach
explains why this simple modification works in the second-
order system, as it is equivalent to the lowest order slimplectic
GGL method (see also Lew et al. 2004 for a similar Lagrange–
de Almambert approach). The slimplectic method allows this to be

\[
\frac{\partial L_d}{\partial q_{n+1/2}} - \frac{\partial L_d}{\partial q_{n-1/2}} \right\}_{\text{PL}} = 0.
\]

\[
\frac{\partial L_d}{\partial q_{n+1/2}} - \frac{\partial L_d}{\partial q_{n-1/2}} \right\}_{\text{PL}} = 0.
\]

\[
\frac{\partial L_d}{\partial q_{n+1/2}} - \frac{\partial L_d}{\partial q_{n-1/2}} \right\}_{\text{PL}} = 0.
\]
generalized to higher orders and general nonconservative systems.8

4. CODE AND EXAMPLES

We have developed a simple python code, slimplectic, that is publicly available9 and generates the fixed-time-step slimplectic GGL integrators described above, for use in characterizing the numerical technique. The code generates slimplectic solvers of arbitrary order \((2r + 2)\) given sympy (SymPy Dev Team 2014) expressions for \(L(q, \dot{q}, t)\) and \(K(q, \dot{q}, r)\). This demonstration code is designed to work for arbitrary \(L\) and \(K\), and thus has not been optimized as would be appropriate for specific problems. In particular, the equations of motion (13) are solved with standard root-finders, rather than a problem-specific iteration method, to be more generally applicable.

As a basic example in Figure 2 we compare Runge–Kutta (RK) and slimplectic integration of a simple damped harmonic oscillator, for both second- and fourth-order methods. Below we also present two basic astrophysical examples of non-conservative interactions. All examples are available as ipython notebooks in our public repository.9

4.1. Poynting–Robertson Drag

We first examine the orbital motion of a dust particle experiencing Poynting–Robertson drag (Burns et al. 1979) due to radiation from a solar type star, starting with a semimajor axis of 1 AU in an eccentric \((e = 0.2)\) orbit. The Lagrangian for this system is

\[
L = \frac{1}{2}m\dot{q}^2 + (1 - \beta) \frac{GM_\odot m}{|q|},
\]

where \(m\) is the dust particle’s mass, and \(q\) its position. The dimensionless factor

\[
\beta \equiv \frac{3L_\odot}{8\pi c\rho GM_\odot d}
\approx 0.058 \left(\frac{\rho}{2 \text{ g cm}^{-3}}\right)^{-1} \left(\frac{d}{10^{-3} \text{ cm}}\right)^{-1}
\]

is the ratio between forces due to radiation pressure and gravity, where \(L_\odot\) and \(M_\odot\) are the solar luminosity and mass, \(\rho\) and \(d\) are the density and size of the dust grain. The nonconservative potential which generates the correct Poynting–Robertson drag force is \((|q| \ll c)\) found as the virtual work from the known force,

\[
K = -\frac{\beta GM_\odot m}{c q^2} \times \left[ \dot{q}_+ \cdot q_- + \frac{1}{q_+} (\dot{q}_+ \cdot \dot{q}_-) (\dot{q}_- \cdot q_-) \right].
\]

Methods to determine or derive \(K\) are discussed in (Galley et al. 2014). The first term in square brackets above gives the usual drag term, while the second term is due to the Doppler shift caused by radial motion.

The system was integrated for 6000 years using second- and fourth-order RK (green and blue dashed) and slimplectic (red and orange solid) methods with time steps of \(\Delta t = 0.01\) year. The results and discussion are shown in Figure 3.

4.2. Gravitational Radiation Reaction

We also consider two \(1.4M_\odot\) neutron stars inspiraling from gravitational wave emission. This example demonstrates (fixed-time-step) integrators for systems where the orbital dynamics can change quickly due to nonconservative effects. In the post-Newtonian (PN) approximation, leading-order conservative dynamics for the orbital separation, \(q\), are described by Newtonian gravity

\[
L = \frac{1}{2} \mu \dot{q}^2 + \frac{\mu M}{|q|},
\]

where \(M = m_1 + m_2 = 2.8M_\odot\) is the total mass, \(\mu = m_1 m_2 / M = 0.7M_\odot\) is the reduced mass, and \(G = c = 1\). Dissipative effects from radiation reaction first appear at PN order \((|q|/c)^5\) (or 2.5PN) and are described by \(K\), which has been calculated in Galley & Leibovich (2012) and Galley &

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Figure 3. Top: evolution of the Cartesian x-coordinate for orbital motion of a particle experiencing Poynting–Robertson drag due to radiation from a solar-type star, with particle density \(\rho = 2 \text{ g cm}^{-3}\) and particle size \(d = 5 \times 10^{-2}\) cm. The particle has initial semimajor axis of 1 AU, and initial eccentricity of 0.2. With a fixed-time-step of \(\Delta t = 0.01\) year, the second-order RK integrator (green-dashed) is unstable, while the second-order slimplectic integrator (red) behaves much more accurately, despite significant (numerical) precession over a \(\sim 1000\) year timescale. The fourth-order integrators (RK, blue-dashed; slimplectic, orange) have similar long-term amplitude evolution without visible numerical precession. The phase errors (not shown) of the RK integrators grow \(\propto t\), while the slimplectic integrators have phase error \(\propto \dot{t}\) (see Preto & Tremaine 1999). Bottom: fractional energy error (compared to a sixth-order slimplectic integration) for the system described above. The RK errors grow roughly linearly in time, while the slimplectic errors are bounded. There is a slight turn-up in the fourth-order slimplectic error envelope, most likely due to the build up of round-off, bias, or action-discretization error.
Figure 4. Top: PN radiation reaction, including only the 2.5PN dissipative terms through $K$. Each of the methods (RK and simplectic GGL) are fourth-order with fixed time steps of $\Delta t = 1000M$ and $\Delta M = T_{\text{ISCO}}$. The integration methods blow up when the orbital timescale is comparable to the time step, though the simplectic method performs significantly better than the RK method for the same time steps; for the 1000M time step the RK method is immediately unstable. Bottom: relative error in the orbital radius compared to the analytic adiabatic-approximation solution.

Figure 5. Top: the phase evolution of the integrators for the PN radiation reaction depicted in Figure 4. Bottom: absolute orbital-phase errors. In this example, both simplectic integrators (phase error $\propto t$), track the orbital phase much better than the equivalent RK integrators (phase error $\propto t^2$).

5. DISCUSSION

We have developed a new method of numerical integration that combines the nonconservative action principle of Galley (2013) and Galley et al. (2014) with the variational-integrator approach of Marsden & West (2001). These “simplectic” integrators allow nonconservative effects to be included in the numerical evolution, while still possessing the major benefits of normally conservative symplectic integrators, particularly the accurate long-term evolution of momenta and energy.

The discrete equations of motion are found by varying a discretized nonconservative action and implicitly defining the simplectic mapping $q_{n+1} \to (q_{n+1}, \tau_{n+1})$. Different choices of discretization generate different variational integrators. Here we have focused on implementing the GGL discretization, and demonstrating its long-term accuracy using the damped harmonic oscillator, Poynting–Robertson drag on a small particle, and a gravitational radiation-reaction toy problem.
Our results also explain why the modification of the second-order “kick-drift-kick” ansatz to include dissipative forces performs so accurately, as this is equivalent to the lowest-order version of the simplectic GGL method.

We have developed a demonstration python code, slimplectic,\(^9\) which generates simplectic integrators for arbitrary Lagrangians and nonconservative potentials. Readers are encouraged to test different physical systems of interest using this publicly available code, but to separately implement problem specific optimizations, particularly when solving the implicit equations of motion.

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