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Variational integrators and the Newmark algorithm for conservative and dissipative mechanical systems

C. Kane[1,‡], J. E. Marsden[2,*,†], M. Ortiz[1,§] and M. West[2,¶]

[1] *Graduate Aeronautical Laboratories and CDS, California Institute of Technology, Pasadena, CA 91125, U.S.A.*
[2] *CDS 107-81, California Institute of Technology, Pasadena, CA 91125, U.S.A.*

SUMMARY

The purpose of this work is twofold. First, we demonstrate analytically that the classical Newmark family as well as related integration algorithms are variational in the sense of the Veselov formulation of discrete mechanics. Such variational algorithms are well known to be symplectic and momentum preserving and to often have excellent global energy behaviour. This analytical result is verified through numerical examples and is believed to be one of the primary reasons that this class of algorithms performs so well.

Second, we develop algorithms for mechanical systems with forcing, and in particular, for dissipative systems. In this case, we develop integrators that are based on a discretization of the Lagrange d'Alembert principle as well as on a variational formulation of dissipation. It is demonstrated that these types of structured integrators have good numerical behaviour in terms of obtaining the correct amounts by which the energy changes over the integration run. Copyright © 2000 John Wiley & Sons, Ltd.

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1. INTRODUCTION AND BACKGROUND

1.1. Overview

We begin with the following intriguing quote from Simo *et al.* [1]:

> What may seem surprising is that all of the implicit members of the Newmark family, perhaps the most widely used time-stepping algorithms in nonlinear structural dynamics, *are not designed to conserve energy and also fail to conserve momentum*. Among the explicit members, only the central difference method preserves momentum.

*Correspondence to: J.E. Marsden, California Institute of Technology, Control and Dynamical Systems 107-81, Pasadena, CA 91125, U.S.A.
†E-mail: marsden@cds.caltech.edu
‡E-mail: kane@cds.caltech.edu
§E-mail: ortiz@madrid.caltech.edu
¶E-mail: mwest@cds.caltech.edu

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Rather little has been done on the analysis and structure of the Newmark family since this work of Simo, Tarnow and Wong (some earlier literature is reviewed in Section 3). The present paper aims to fill this gap. The key to our approach is the recent progress in variational integrators based on the Veselov theory of discrete mechanics and the inclusion of dissipation and forcing into these schemes using optimization techniques.

We shall show (in a sense that is not entirely obvious) that the classical Newmark scheme is indeed variational and so is symplectic and momentum preserving. This appears, at first sight, to contradict the above quote. This apparent paradox is resolved by realizing that the construction of the conserved symplectic form and the momentum is not done in a completely obvious way, and thus it is a non-canonical symplectic form and non-standard momenta that are conserved.

It is known that symplectic integrators often have remarkable near energy preserving properties and we believe that the symplectic nature of the Newmark scheme goes a long way towards explaining its excellent performance, often better than that of high-order schemes for moderately long-time integrations of conservative and forced systems (see, for example, References [2, 3] and references therein). We shall present specific examples of this phenomenon in this paper.

Main results of this paper: The main accomplishments of the present paper are:

1. We show the precise sense in which the Newmark algorithm is variational.
2. As a consequence of its variational nature, the Newmark scheme exactly preserves a certain symplectic structure and a certain algorithmically computed momentum (linear or angular momentum, as appropriate).
3. Dissipation and forcing are incorporated into the Newmark and variational schemes.
4. Numerical tests of these schemes are given for some relatively simple systems to demonstrate their effective performance.

1.2. Background on geometric integrators

1.2.1. Mechanical integrators There is a large literature that has developed on the use of energy–momentum and symplectic–momentum integrators. For time stepping algorithms with fixed time steps, the theorem of Ge and Marsden [4] led to a general division of algorithms into those that are energy–momentum preserving and those that are symplectic–momentum preserving.

If one takes a spacetime view of variational integrators, as is advocated in Reference [5], then one can have integrators that preserve the energy, momentum and the symplectic structure, as has been shown in Reference [6]. Papers typified by Simo and Tarnow [7], Simo *et al*. [1] and Gonzalez [8] have focussed on energy preserving algorithms, but they presumably fail (except, perhaps, in special cases, such as integrable systems) to be symplectic. For a survey of other literature, see Reference [9].

1.2.2. Accuracy of solutions It is well known that structure preservation alone does not guarantee accuracy of individual trajectories (see, e.g., References [10, 11]). Complicating this issue is the fact that for systems with complicated, unstable, or chaotic trajectories, accuracy of individual trajectories is presumably not the correct question to ask. Rather one should probably concentrate on accurate prediction of statistical or stably reproducible properties of solution families. However, as has been frequently demonstrated and we shall do so here as well, in many circumstances structure preserving algorithms often perform remarkably well—far better than an error analysis would suggest.

One also must be cautious here. When the time steps are too large, symplectic schemes may have bad energy behaviour and fail to be accurate. See, for example, Reference [12]. Consistent with this, it is also known that the Newmark method can perform badly on some nonlinear systems with moderately large time steps, and it is certainly not unconditionally stable. The results in this paper do not contradict this, as our results hold only for sufficiently small timesteps, and do not address the short term stability bounds of the integrators. We discuss this issue further in Section 3.

1.2.3. Discrete Lagrangian mechanics and integrators Veselov [13] developed a discrete version of Lagrangian mechanics with an emphasis on variational methods (see also Reference [14]). In particular, he showed, as in the theory of generating functions, that the corresponding discrete Euler–Lagrange equations define symplectic maps. Using these ideas, it can be shown that several well-known algorithms, such as the Verlet and shake methods, are variational integrators (see References [15, 16]). There have been considerable additional efforts in this area, such as Marsden *et al.* [5], Kane *et al.* [6], Marsden *et al.* [17, 18] Bobenko *et al.* [19], and Bobenko and Suris [20]. We shall comment on some of the related developments below and in the body of the paper.

In structural mechanics, the $\beta = 0,\ \gamma = 1/2$ (central differences) member of the widely used Newmark family has been known to be symplectic and momentum preserving for some time (see, for example, Reference [1]). This was shown by more or less ad hoc techniques as a 'curious observation'. One of our main results is to extend this to all members of the Newmark family (for unforced mechanical systems with $\gamma = 1/2$). We shall do this by showing that *the Newmark algorithm is indeed variational in the sense of Veselov*.

1.2.4. Dissipation A second main point of this paper is to demonstrate the effectiveness of variational techniques for dissipative or more generally, forced mechanical systems. One possibility is that dissipative effects can be dealt with by means of product formulas, as in References [21–23]. Another is to incorporate the dissipative effects into the variational principle, as in Reference [24] (see also Reference [25]). We shall abstract some of these techniques in this paper.

1.2.5. Constraints Constraints are of obvious importance for integrators. We do not discuss these in any detail in this paper. However, we do mention that variational integrators usually handle constraints in a simple and efficient way using Lagrange multipliers, as shown in, for example, Reference [16]. In addition, when handled variationally, constraints do not disturb the symplectic or conservative nature of the algorithms. It is well known that other techniques can run into trouble in this regard. See, for example, the discussion of this point in Reference [26].

1.2.6. Multisymplectic integrators Variational methods also generalize to pde's using multisymplectic geometry with the result being a class of multisymplectic momentum integrators. See Reference [5] for details and numerical examples; see also Reference [27]. This type of approach should ultimately be of use in elastodynamics as well as ocean dynamics, for example.

1.2.7. Symmetry and reduction We should also mention that for mechanical systems with symmetry, the investigation of discrete versions of reduction theory, such as Euler–Poincaré reduction are of current interest (see, for example, References [17, 18]). We will not be making use of this reduction theory in this paper, but this work is related since our integrators are intended to preserve symmetry.

2. VARIATIONAL INTEGRATORS

2.1. A review of variational integrators

2.1.1. Variational algorithms Variational schemes following the Veselov discretization technique are now well known and we briefly review them here. See, for example, References [5, 6, 15–18].

These schemes are known to be automatically symplectic (and are often second-order accurate) integrators that preserve conserved quantities (such as linear and angular momentum) associated with symmetries provided the discrete Lagrangian has these symmetries.

We briefly recall these schemes here. Given a configuration space Q, a *discrete Lagrangian* is a map

$$L_{\mathrm{d}} : Q \times Q \to \mathbb{R}$$

In practice, L_{d} is obtained by approximating the action function associated with a given Lagrangian as we shall discuss later, but regard L_{d} as given for the moment. The time step information will be contained in L_{d} and we regard L_{d} as a function of two nearby points (q_k, q_{k+1}).

Example. Consider a continuous Lagrangian of the standard form

$$L(q, \dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}} M \dot{q} - V(q) \tag{1}$$

where M is a symmetric positive-definite mass matrix, $q \in \mathbb{R}^n = Q$ and V is a given potential. Define an associated *discrete Lagrangian*, $L_{\mathrm{d}}^{\alpha} : Q \times Q \to \mathbb{R}$ by

$$L_{\mathrm{d}}^{\alpha}(q_0, q_1) = hL\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right) \tag{2}$$

where $h \in \mathbb{R}_+$ is the time step and $0 \leqslant \alpha \leqslant 1$ is an interpolation parameter. Using the given form of L, this becomes

$$L_{\mathrm{d}}^{\alpha}(q_0, q_1) = h\frac{1}{2}\left(\frac{q_1 - q_0}{h}\right)^{\mathrm{T}} M\left(\frac{q_1 - q_0}{h}\right) - hV((1-\alpha)q_0 + \alpha q_1) \tag{3}$$

We shall return to a systematic study of discrete Lagrangians of this form shortly in Section 2.2.

For a positive integer N, the *action sum* is the map $S_{\mathrm{d}} : Q^{N+1} \to \mathbb{R}$ defined by

$$S_{\mathrm{d}} = \sum_{k=0}^{N-1} L_{\mathrm{d}}(q_k, q_{k+1}) \tag{4}$$

where $q_k \in Q$ and k is a non-negative integer. The action sum is the discrete analog of the action integral

$$S = \int_a^b L(q(t), \dot{q}(t))\,\mathrm{d}t \tag{5}$$

The *discrete variational principle* states that the evolution equations extremize the action sum given fixed end points, q_0 and q_N. Extremizing S_{d} over $q_1, \ldots, q_{N-1}$ leads to the *discrete Euler–Lagrange* (DEL) *equations*:

$$D_1 L_{\mathrm{d}}(q_{k+1}, q_{k+2}) + D_2 L_{\mathrm{d}}(q_k, q_{k+1}) = 0 \tag{6}$$

for all $k = 1, \ldots, N-1$, where $D_1 L$ denotes the derivative of L with respect to its first slot. We can write this equation in terms of a discrete algorithm:

$$\Phi : Q \times Q \to Q \times Q$$

defined implicitly by

$$D_1 L_{\mathrm{d}} \circ \Phi + D_2 L_{\mathrm{d}} = 0$$

i.e.

$$\Phi(q_k, q_{k+1}) = (q_{k+1}, q_{k+2})$$

If, for each fixed $q \in Q$, the map $D_1 L_{\mathrm{d}}(q,q) : T_q Q \to T_q^* Q$ is invertible, then $D_1 L_{\mathrm{d}} : Q \times Q \to T^* Q$ is locally invertible in a neighbourhood of the diagonal and so the algorithm Φ is well defined for small time steps.

Example. For the discrete Lagrangian (2), the DEL equations are readily computed to be

$$\frac{M}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = -(1-\alpha)\nabla V((1-\alpha)q_{k+1} + \alpha q_{k+2}) - \alpha \nabla V((1-\alpha)q_k + \alpha q_{k+1}) \tag{7}$$

This specific example will play an important role in subsequent sections of the paper.

2.1.2. Variational algorithms are symplectic To explain the sense in which the algorithm is symplectic, first define the *fibre derivative* (or the discrete Legendre transform) by

$$\mathbb{F}L_{\mathrm{d}} : Q \times Q \to T^* Q; \quad (q_0, q_1) \mapsto (q_1, D_2 L_{\mathrm{d}}(q_0, q_1)) \tag{8}$$

and define the 2-form $\Omega_{L_{\mathrm{d}}}$ on $Q \times Q$ by pulling back the canonical 2-form $\Omega = \mathrm{d}q^i \wedge \mathrm{d}p_i$ from $T^* Q$ to $Q \times Q$:

$$\Omega_{L_{\mathrm{d}}} = (\mathbb{F}L_{\mathrm{d}})^*(\Omega)$$

The alternative discrete fibre derivative $\tilde{\mathbb{F}}L_{\mathrm{d}}(q_0, q_1) := (q_0, -D_1 L_{\mathrm{d}}(q_0, q_1))$ may be used and the results obtained will be essentially unchanged. Either definition may be regarded as an analog of the standard Legendre transform

$$\mathbb{F}L : TQ \to T^* Q; \quad (q, \dot{q}) \mapsto (q, D_2 L(q, \dot{q})) \tag{9}$$

An expression for $\Omega_{L_{\mathrm{d}}}$ in terms of the co-ordinates q_0^i, q_1^i of the points q_0, q_1 is

$$\Omega_{L_{\mathrm{d}}} = \frac{\partial^2 L_{\mathrm{d}}}{\partial q_0^i \partial q_1^j}(q_0, q_1)\, \mathrm{d}q_0^i \wedge \mathrm{d}q_1^j$$

A fundamental fact is that *the algorithm* Φ *exactly preserves the symplectic form* $\Omega_{L_{\mathrm{d}}}$. That is, $\Phi^* \Omega_{L_{\mathrm{d}}} = \Omega_{L_{\mathrm{d}}}$.

One proof of this is to simply verify it with a straightforward calculation—see Reference [16] for the details. Another approach is to derive the same conclusion directly from the variational structure, as is done in Reference [5]. This value of this latter approach is particularly apparent when one wishes to consider extensions to variable time-step schemes, as in Reference [6] and to problems involving collisions as in References [28, 29].

2.1.3. The algorithm preserves momentum Recall that *Noether's theorem* states that a continuous symmetry of the Lagrangian leads to conserved quantities, such as linear and angular momentum. One can directly derive these conservation laws using the *invariance of the variational principle* (this is the way Noether originally did it).

Assume that the discrete Lagrangian is invariant under the action of a Lie group G on Q, and let $\xi \in \mathfrak{g}$, the Lie algebra of G. By analogy with the continuous case, define the *discrete momentum map*, $\mathbf{J}_{\mathrm{d}} : Q \times Q \to \mathfrak{g}^*$ by

$$\langle \mathbf{J}_{\mathrm{d}}(q_k, q_{k+1}), \xi \rangle := \langle D_2 L_{\mathrm{d}}(q_k, q_{k+1}), \xi_Q(q_{k+1}) \rangle \tag{10}$$

A second fundamental fact is that *the algorithm* Φ *exactly preserves the momentum map*.

Example. Consider a Lagrangian of the usual kinetic minus potential energy form as above:

$$L(q, \dot{q}) = \tfrac{1}{2} \dot{q}^{\mathrm{T}} M \dot{q} - V(q)$$

and the discrete Lagrangian (2). Assume that V is independent of q^1 so that $p_1 = [M\dot{q}]_1$ (the first component of $M\dot{q}$) is a constant of the motion for the continuous system (q^1 is a cyclic variable).

The corresponding conserved discrete momentum map given by (10) is the algorithmic analog of the momentum in the first co-ordinate direction (notice that the time step h cancels in the calculation):

$$J_{\mathrm{d}}(q_k, q_{k+1}) = [M(q_{k+1} - q_k)]_1$$

Being a constant of the motion means that $J_{\mathrm{d}}(q_k, q_{k+1})$ is independent of k. One of course can verify this directly, but it is guaranteed by the theory. Related examples such as linear and angular momentum for systems of particles or rigid bodies proceed in a similar way.

2.1.4. Associated energy The energy function associated to a given discrete Lagrangian is defined, according to Kane *et al.* [6], by

$$E_{\mathrm{d}}(q_0, q_1, h) = -\frac{\partial}{\partial h}[L_{\mathrm{d}}(q_0, q_1, h)] \tag{11}$$

where the time step has been inserted explicitly into the discrete Lagrangian in its third variable slot. One can motivate this definition of the energy using the variational principle and this definition may be viewed as a discrete form of the Hamilton–Jacobi equation.

Example. For the discrete Lagrangian (2), the associated discrete energy is easily verified to be

$$E_{\mathrm{d}}^{\alpha}(q_0, q_1, h) = \frac{1}{2} \left(\frac{q_1 - q_0}{h} \right)^{\mathrm{T}} M \left(\frac{q_1 - q_0}{h} \right) + V((1 - \alpha) q_0 + \alpha q_1) \tag{12}$$

In this example, we can write this as

$$E_{\mathrm{d}}^{\alpha}(q_0, q_1, h) = E\left((1 - \alpha) q_0 + \alpha q_1, \left(\frac{q_1 - q_0}{h} \right) \right) \tag{13}$$

where $E(q, \dot{q})$ is the energy function associated with the original Lagrangian $L(q, \dot{q})$.

2.2. Construction of mechanical integrators

Assume we have a mechanical system defined by a Lagrangian $L : TQ \to \mathbb{R}$. If Q is an arbitrary manifold, then one typically proceeds by embedding it within a vector space and treating Q as a constraint manifold. We will assume for simplicity that Q is a linear space.

We regard the discrete action sum (4) as an approximation to the action integral (5). Therefore, it is natural to choose the discrete Lagrangian $L_\mathrm{d} : Q \times Q \to \mathbb{R}$ to be an approximation

$$L_\mathrm{d}(q_0, q_1) \approx \int_0^h L(q(t), \dot{q}(t))\,\mathrm{d}t$$

where $q(t)$ is a true trajectory of the system that moves from q_0 at time $t = 0$ to q_1 at time $t = h$. The right-hand side, of course, is Jacobi's form of the exact solution $S(q_0, q_1, h)$ of the Hamilton–Jacobi equation.

We have already introduced one important class of discrete Lagrangians, namely L_d^α in Equation (2). Another class of examples will be introduced below.

We introduce the useful *evaluated acceleration notation*:

$$a_{k+\alpha} := M^{-1}[-\nabla V((1-\alpha)q_k + \alpha q_{k+1})] \tag{14}$$

With this notation, the algorithm (7) reads

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = (1-\alpha)a_{k+1+\alpha} + \alpha a_{k+\alpha} \tag{15}$$

This is a second-order accurate implicit algorithm on $Q \times Q$. For a Lagrangian not of the special form above this need only be a first-order accurate algorithm for general α, but is second-order accurate for $\alpha = 1/2$.

A second choice of discrete Lagrangian is a symmetric version of the expression (2) for L_d^α, defined by

$$L_\mathrm{d}^{\mathrm{sym},\alpha}(q_0, q_1) = \frac{h}{2} L\left((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\right) + \frac{h}{2} L\left(\alpha q_0 + (1-\alpha)q_1, \frac{q_1 - q_0}{h}\right) \tag{16}$$

where, once again, $h \in \mathbb{R}^+$ is the time step and $\alpha \in [0, 1]$ is a real parameter.

For this discrete Lagrangian the corresponding discrete Euler–Lagrange equations also have a symmetric form. For L given by (1) and using the evaluated acceleration notation (14), the DEL equations are

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = \frac{1}{2}(1-\alpha)a_{k+1+\alpha} + \frac{1}{2}\alpha a_{k+2-\alpha} + \frac{1}{2}\alpha a_{k+\alpha} + \frac{1}{2}(1-\alpha)a_{k+1-\alpha} \tag{17}$$

These equations define a second-order accurate, implicit algorithm for any parameter α, and are still second-order accurate if we use an arbitrary Lagrangian L.

Both algorithms (15) and (17), derived from L_d^α and $L_\mathrm{d}^{\mathrm{sym},\alpha}$, respectively, preserve the associated discrete symplectic form Ω_{L_d} and the discrete momentum map. By choosing α correctly these two algorithms recover many schemes known elsewhere under different names. Some examples of this are mentioned below.

2.3. Representations of variational integrators

One may think that the discrete symplectic form and momentum map that are conserved by the variational algorithm are somehow 'concocted' to be conserved. This is not the case. Indeed, one can, via the discrete Legendre transform, transfer the algorithm to position-momentum space. Transferred to these variables, the algorithm will preserve the *standard* symplectic form $\mathrm{d}q^i \wedge \mathrm{d}p_i$ and the *standard* momentum map. If desired, one can then use the continuous Legendre transform to move the algorithm to TQ, where it will once again preserve the standard Lagrangian symplectic two-form Ω_L and the standard momenta.

To state these ideas more clearly, we summarize the three phase spaces we are using.

Phase space	Local co-ords.	Symp. form	Function
T^*Q	(q, p)	Ω	Hamiltonian H
TQ	$(q, \dot{q})$	Ω_L	Lagrangian L
$Q \times Q$	(q_0, q_1)	Ω_{L_d}	Discrete Lagrangian L_d

The standard mappings between the phase spaces given above are

$$\begin{array}{ccc} & & Q\times Q \\ & & \Big\downarrow{\scriptstyle \mathbb{F}L_\mathrm{d}} \\ TQ & \xrightarrow[\mathbb{F}L]{} & T^*Q \end{array}$$

In this section we will be using the symmetric discrete Lagrangian $L_\mathrm{d}^{\mathrm{sym},\alpha}$ and assuming that the Lagrangian L is given by (1). With these definitions the continuous and discrete fibre derivatives given by (9) and (8) have the form

$$\mathbb{F}L(q, \dot{q}) = (q, M\dot{q})$$

$$\mathbb{F}L_\mathrm{d}^{\mathrm{sym},\alpha}(q_0, q_1) = \left(q_1, M\left[\frac{1}{h}(q_1 - q_0) + \frac{h}{2}(\alpha a_{0+\alpha} + (1-\alpha)a_{1-\alpha})\right]\right)$$

2.3.1. The variational algorithm on T^*Q Pushing the variational algorithm (17) forward with $\mathbb{F}L_\mathrm{d}^{\mathrm{sym},\alpha}$ we obtain an implicit algorithm, which we denote

$$(q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$$

given by

$$q_{k+1} = q_k + hM^{-1}p_k + \frac{h^2}{2}[(1-\alpha)a_{k+\alpha} + \alpha a_{k+1-\alpha}]$$

$$p_{k+1} = p_k + hM\left(\frac{1}{2}a_{k+\alpha} + \frac{1}{2}a_{k+1-\alpha}\right)$$

This algorithm is second-order accurate for any α and preserves the canonical symplectic form Ω and the standard momentum map.

Considering the particular case of $\alpha = 1/2$ we see that the above algorithm can be written

$$\frac{1}{h}\begin{pmatrix} q_{k+1} - q_k \\ p_{k+1} - p_k \end{pmatrix} = \begin{pmatrix} M^{-1}\left(\dfrac{p_{k+1} + p_k}{2}\right) \\ -\nabla V\left(\dfrac{q_{k+1} + q_k}{2}\right) \end{pmatrix}$$

which, for $z = (q, p)$, has the more compact representation

$$\frac{z_{k+1} - z_k}{h} = X_H\left(\frac{z_{k+1} + z_k}{2}\right) \tag{18}$$

where X_H is the Hamiltonian vector field corresponding to the Hamiltonian

$$H = \tfrac{1}{2}\, p^{\mathrm{T}} M^{-1} p + V(q)$$

This is the classical midpoint rule.

We summarize the results in the following:

Theorem 2.1. The classical midpoint rule (18) is, via the discrete Legendre transformation, a variational algorithm with the choice $L_{\mathrm{d}} = L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ and $\alpha = 1/2$.

2.3.2. The variational algorithm on TQ Next, we pull the variational algorithm back with $\mathbb{F}L$ from T^*Q to TQ to obtain an algorithm $(q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1})$ given by

$$\begin{aligned} q_{k+1} &= q_k + h\dot{q}_k + \frac{h^2}{2}[(1-\alpha)a_{k+\alpha} + \alpha a_{k+1-\alpha}] \\ \dot{q}_{k+1} &= \dot{q}_k + h(\tfrac{1}{2}a_{k+\alpha} + \tfrac{1}{2}a_{k+1-\alpha}) \end{aligned} \tag{19}$$

This algorithm is second-order accurate for any α and preserves the standard Lagrangian symplectic form Ω_L and the standard momentum map.

Aside from the midpoint rule mentioned above, a number of other classical integrators are also special cases of variational schemes. We get the *shake* algorithm with L_{d}^{α} for $\alpha = 1$ (the *Verlet* algorithm is the unconstrained version of the shake algorithm). The *Moser–Veselov discrete Lagrangian* for the rigid body is constructed using L_{d}^{α} with either $\alpha = 0$ or 1 (see Reference [17, 18] for details).

3. THE NEWMARK ALGORITHM IS VARIATIONAL

The goal of this section is to prove that the Newmark scheme for conservative mechanical systems is variational, and to discuss some of the implications of this fact. The variational nature of the Newmark scheme and its performance is of particular interest because of its widespread use in finite element codes.

3.1. Newmark schemes

We begin with a mechanical system on Euclidean n-space with a Lagrangian of the form

$$L(q,\dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}} M \dot{q} - V(q) \tag{20}$$

where $q, \dot{q} \in \mathbb{R}^n$, M is a constant symmetric and positive-definite mass matrix, and V is a given potential energy.

The corresponding Euler–Lagrange equations are, using vector notation

$$M\ddot{q} = -\nabla V(q) \tag{21}$$

The Newmark family [30] is one of the most widely used algorithms in structural dynamics. General references are Hughes [31] and Geradin and Rixen [32]. This family is usually written in the following way. Let γ and β be real numbers, $0 \leqslant \gamma \leqslant 1$, $0 \leqslant \beta \leqslant 1/2$. Given $(q_k, \dot{q}_k)$, find $(q_{k+1}, \dot{q}_{k+1})$ such that

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}[(1-2\beta)a_k + 2\beta a_{k+1}] \tag{22}$$

$$\dot{q}_{k+1} = \dot{q}_k + h[(1-\gamma)a_k + \gamma a_{k+1}] \tag{23}$$

where we are using the convenient evaluated acceleration notation as earlier, defined by

$$a_k = M^{-1}(-\nabla V(q_k)) \tag{24}$$

We recall that the Newmark algorithm is second-order accurate if and only if $\gamma = 1/2$, otherwise it is only consistent. Thus, one usually chooses $\gamma = 1/2$. If $\beta = 0$ then Equation (22) is an explicit equation for q_{k+1} in terms of $(q_k, \dot{q}_k)$, making the $\beta = 0$ case known as *explicit Newmark*.

Detailed analyses of the Newmark algorithm, its stability and energy preserving properties (for linear systems, $\beta = 114$) were given in Belytschko and Schoeberle [33], Hughes [34] and related papers.

3.1.1. Simple comparison The relationship between the Newmark algorithm and the variational schemes discussed earlier can be clearly seen by comparing the $\alpha = 1/2$, $\beta = 1/4$ Newmark:

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}\left(\frac{a_k + a_{k+1}}{2}\right)$$

$$\dot{q}_{k+1} = \dot{q}_k + h\left(\frac{a_k + a_{k+1}}{2}\right)$$

to the $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ with $\alpha = 1/2$ variational scheme:

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}a_{k+1/2}$$

$$\dot{q}_{k+1} = \dot{q}_k + ha_{k+1/2}$$

Looking at these two equations, we see that Newmark *averages forces*, whereas the variational method *evaluates forces at averaged positions*. We now show that this is not, in fact, an essential difference, and the algorithms are in fact equivalent.

3.1.2. Newmark as an update of configuration points As we have already seen, it is possible to regard variational algorithms either as updates of positions $(q_k, q_{k+1}) \mapsto (q_{k+1}, q_{k+2})$ or as updates of positions and velocities $(q_k, \dot{q}_k) \mapsto (q_{k+1}, \dot{q}_{k+1})$. This is also true of the Newmark algorithm, and to compare these two schemes it will be beneficial to work with both of them in position-update form.

Firstly, note that the velocities in Newmark can be recovered from the positions using (22). This gives

$$\dot{q}_k = \frac{1}{h}(q_{k+1} - q_k) - \frac{h}{2}[(1-2\beta)a_k + 2\beta a_{k+1}]$$

$$\dot{q}_{k+1} = \frac{1}{h}(q_{k+2} - q_{k+1}) - \frac{h}{2}[(1-2\beta)a_{k+1} + 2\beta a_{k+2}]$$

Substituting these two expressions into the velocity update Equation (23) and rearranging we obtain an explicit expression reminiscent of that for the variational algorithm:

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) - \beta a_{k+2} + (2\beta - \gamma - 1/2)a_{k+1} + (-\beta + \gamma - 1/2)a_k = 0 \tag{25}$$

3.1.3. Equivalence of Newmark and variational schemes We will explore three ways in which the Newmark and variational schemes can be regarded as equivalent:

1. For certain parameter values, or for linear systems, the Newmark algorithm is the same as the transformation of the variational algorithm corresponding to $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ from $Q \times Q$ to TQ using the Legendre transformations for $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ and L.
2. Under *much more general assumptions*, we will show that *any* Newmark trajectory with $\gamma = 1/2$ and $\beta \leqslant 1/4$ is *shadowed*, in a sense we will make precise, by a trajectory of a variational algorithm.
3. Finally, we will establish that *any Newmark algorithm with* $\gamma = 1/2$ is *directly* variational. That is, we will construct a discrete Lagrangian L_{d}^{β} for which the discrete Euler–Lagrange equations are the Newmark method for $\gamma = 1/2$ and the given β.

We will cover each type of equivalence in turn. The first way is more elementary, direct, and to some extent known. Of primary interest are the second and third methods, but we include the first for completeness and for motivation.

3.2. Central differences and linear systems

We shall start the process of proving that Newmark is variational with the well known cases when $\beta = 0$ and $\gamma = 1/2$, or any Newmark scheme with $\gamma = 1/2$ and $\beta \leqslant 1/4$ for a linear system.

Theorem 3.1. The Newmark algorithm with $\beta = 0$ and $\gamma = 1/2$ is the same as the variational algorithm derived from $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ with $\alpha = 0$ or 1 pushed forward to TQ with the discrete Legendre transform.

Proof. Substituting the specified parameters into the Newmark equations (22) and (23), and into the variational equations on TQ (19) we see that in both cases we obtain

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}a_k$$

$$\dot{q}_{k+1} = \dot{q}_k + h(\tfrac{1}{2}a_k + \tfrac{1}{2}a_{k+1})$$

and thus have equivalence. □

3.2.1. Linear systems One can say a little more in the case of linear systems, that is, in the case of quadratic potentials. This is interesting because of the long history of Newmark in the linear finite element literature.

Theorem 3.2. For potentials V so that ∇V is affine, Newmark with $\gamma = 1/2$ and any $\beta \leqslant 1/4$ is the same as the $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ variational algorithm when α is chosen so that $\beta = \alpha(1-\alpha)$.

A special case of this is the variational nature of the (*constant*) *average acceleration method* ($\beta = 1/4,\ \gamma = 1/2$) which is equivalent to the $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ ($\alpha = 1/2$) variational algorithm.

Proof. Once again this is a simple verification. For affine ∇V we have that $a_{k+\alpha} = (1-\alpha)a_k + \alpha a_{k+1}$ and substituting this into the variational Equation (19) and rearranging we obtain

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}((1 - 2[\alpha(1-\alpha)])a_k + 2[\alpha(1-\alpha)]a_{k+1})$$

$$\dot{q}_{k+1} = \dot{q}_k + h(\tfrac{1}{2}a_k + \tfrac{1}{2}a_{k+1})$$

which is Newmark for $\beta = \alpha(1-\alpha)$ and $\gamma = 1/2$. For any given $\beta \leqslant 1/4$ there is clearly an α so that $\beta = \alpha(1-\alpha)$. □

3.3. Shadowing of Newmark trajectories

We will now turn to a much more general class of Newmark algorithms and consider their action upon general non-linear systems. In both this section and the next we are concerned with Newmark algorithms with the parameter γ equal to $1/2$.

This assumption is not as restrictive as it may initially appear. It is well known (see, for example, Reference [31]) that with $\gamma < 1/2$ Newmark numerically dissipates energy and with $\gamma > 1/2$ it numerically increases energy. For this reason one would not expect that Newmark with $\gamma \neq 1/2$ would be symplectic, and hence not variational.

The first way in which we establish the variational nature of Newmark is to show that any $\gamma = 1/2,\ \beta \leqslant 1/4$ Newmark trajectory will be shadowed by a variational trajectory, and vice versa. By this, we mean that there is some parameter α so that each point x_k of the Newmark trajectory is equal to the interpolation $(1-\alpha)q_k + \alpha q_{k+1}$ of two points $q_k,\ q_{k+1}$ of the variational trajectory. This can be clearly seen in Figure 1, which shows a Newmark and a variational trajectory shadowing each other.

In this section we will always use x_k to denote points on a Newmark trajectory and q_k to denote points on a variational trajectory. In this equivalence we are only interested in the trajectories in

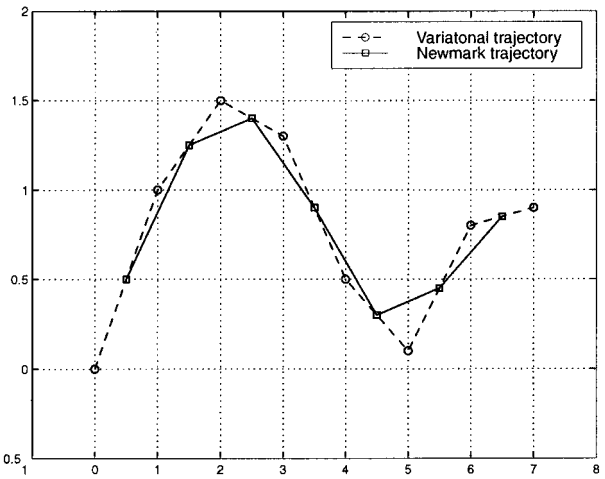

Figure 1. A Newmark trajectory (solid line) and its 'shadow' variational trajectory (dashed line).

configuration space Q and do not consider the velocities. The reason this is possible is that Newmark can be regarded as a position-update only algorithm, as discussed in Section 3.1.

We now give a lemma containing the fundamental fact behind the shadowing variational nature of Newmark.

Lemma 3.3. For any q_0, q_1, q_2 and q_3 lying on a trajectory of the L_d^α variational algorithm for some α, the points x_0, x_1 and x_2 formed by

$$x_k = (1-\alpha)q_k + \alpha q_{k+1}$$

satisfy the position-update Newmark algorithm with $\beta = \alpha(1-\alpha)$ and $\gamma = 1/2$.

Proof. Begin by noting that, by assumption, the two triples (q_0, q_1, q_2) and (q_1, q_2, q_3) both satisfy the discrete Euler–Lagrange equations (15).

Now substitute the expressions for x_k and $\beta = \alpha(1-\alpha)$ into the left-hand side of the position-update Newmark algorithm (25) to obtain

$$\frac{M}{h^2}(-\alpha q_3 + (3\alpha - 1)q_2 + (2 - 3\alpha)q_1 + (\alpha - 1)q_0) - \alpha(1-\alpha)DV((1-\alpha)q_2 + \alpha q_3)$$

$$-(2\alpha^2 - 2\alpha + 1)DV((1-\alpha)q_1 + \alpha q_2) - \alpha(1-\alpha)DV((1-\alpha)q_0 + \alpha q_1)$$

This expression can be rearranged to give

$$= \alpha\left[\frac{M}{h^2}(-q_3 + 2q_2 - q_1) - (1-\alpha)DV((1-\alpha)q_2 + \alpha q_3) - \alpha DV((1-\alpha)q_1 + \alpha q_2)\right]$$

$$+(1-\alpha)\left[\frac{M}{h^2}(-q_2 + 2q_1 - q_0) - (1-\alpha)DV((1-\alpha)q_1 + \alpha q_2) - \alpha DV((1-\alpha)q_0 + \alpha q_1)\right]$$

Each of the bracketed expressions is just the discrete Euler–Lagrange equations satisfied by the sets q_1, q_2, q_3 and q_0, q_1, q_2, and thus the entire expression is zero, as claimed. □

Theorem 3.4. Taking $\gamma = 1/2$, given any parameter β with $0 \leqslant \beta \leqslant 1/4$ and any initial conditions $(x_0, \dot{x}_0)$ for Newmark, there exists, for small time steps h, initial conditions (q_0, q_1) and parameter α for the L_{d}^{α} variational algorithm so that the Newmark and variational trajectories are related by $x_k = (1-\alpha)q_k + \alpha q_{k+1}$ for all k. That is, the trajectories shadow each other for all time.

Conversely, given a parameter α and initial conditions (q_0, q_1) for the L_{d}^{α} variational algorithm, there exists initial conditions $(x_0, \dot{x}_0)$ and parameter β so that the same conclusion holds.

Proof. The proof of this result is essentially a repeated application of the preceding lemma as time increases. The parameters α and β must always be taken so that $\beta = \alpha(1-\alpha)$. Note that this implies two possible values of α for any given $\beta \leqslant 1/4$, except for the 'midpoint' case $\beta = 1/4$ and $\alpha = 1/2$.

Given initial conditions $(x_0, \dot{x}_0)$ for Newmark, compute $(x_1, \dot{x}_1)$ with one step of Newmark. Now we must find q_0, q_1 and q_2 so that

$$\begin{aligned} D_1 L_{\mathrm{d}}^{\alpha}(q_1, q_2) + D_2 L_{\mathrm{d}}^{\alpha}(q_0, q_1) &= 0 \\ (1-\alpha)q_0 + \alpha q_1 &= x_0 \\ (1-\alpha)q_1 + \alpha q_2 &= x_1 \end{aligned}$$

This is done by the implicit function theorem. First, note that if we multiply the first equation by h so that it is regular at $h = 0$, then for $h = 0$, we have the trivial solution $x_0 = x_1 = q_0 = q_1 = q_2$. Now we linearize around this solution; the relevant Jacobian determinant is computed at this solution to be $(1+\alpha^2)\det M$, which is not zero, so we have solvability for small h.

For the converse, given (q_0, q_1), step once with the variational algorithm to find q_2. Form x_0 and x_1 by interpolation and then use the position Equation (22) of Newmark to find $\dot{x}_0$. That is,

$$x_0 = \frac{1}{h}(x_1 - x_0) - \frac{h}{2}[(1-2\beta)a_0 + 2\beta a_1]$$

This completes the proof of the shadowing variational nature of the Newmark scheme. □

It may appear at first that the properties of the variational algorithm will not be inherited by the Newmark method, as we have only established equivalence of the position-update forms of the algorithms in a shadowing sense. In fact, we can regard the 'shadowing' of trajectories as an implicitly defined non-linear co-ordinate change, and the transformation $(q_k, q_{k+1}) \mapsto (q_k, \dot{q}_k)$ for both Newmark and the variational method is also simply a co-ordinate change. Thus, we have that the Newmark and variational algorithms are simply the co-ordinate transformed versions of each other. The advantage in the shadowing result is that it provides clear physical insight into the relationship between the simple L_{d}^{α} variational algorithm and Newmark.

3.4. Newmark itself is variational

Now, we are ready to show the sense in which Newmark itself is directly variational, and thus symplectic and momentum conserving, for $\gamma = 1/2$.

This technique was suggested by Y.B. Suris, who made a key remark to us after viewing an early version of this work. We are most grateful to him for the elegant method of constructing a discrete Lagrangian which generates the Newmark algorithm.

To construct a discrete Lagrangian for $\gamma = 1/2$ Newmark, we begin by noting that for $\gamma = 1/2$ the position-update form of Newmark (25) can be written

$$\frac{1}{h}[(q_{k+2} - \beta h^2 M^{-1}\nabla V(q_{k+2})) - 2(q_{k+1} - \beta h^2 M^{-1}\nabla V(q_{k+1})) + (q_k - \beta h^2 M^{-1}\nabla V(q_k))] + hM^{-1}\nabla V(q_{k+1}) = 0 \tag{26}$$

Making the co-ordinate change $q_k \mapsto x_k = \eta^\beta(q_k)$ defined by

$$x_k = \eta^\beta(q_k) = q_k - \beta h^2 M^{-1}\nabla V(q_k)$$

and introducing a modified potential $\tilde{V}(x_k)$, we can write Newmark as

$$\frac{1}{h}(x_{k+2} - 2x_{k+1} + x_k) + hM^{-1}\nabla \tilde{V}(x_k) = 0 \tag{27}$$

where we require that $\tilde{V}(x_k)$ is related to $V(q_k)$ by

$$\nabla \tilde{V}(x_k) = \nabla V(q_k)$$

for $x_k = \eta^\beta(q_k)$. Equation (27), however, is simply the discrete Euler–Lagrange equations for the discrete Lagrangian

$$L_{\mathrm{d}}(x_0, x_1) = h\frac{1}{2}\left(\frac{x_1 - x_0}{h}\right)^{\mathrm{T}} M\left(\frac{x_1 - x_0}{h}\right) - h\tilde{V}(x_0)$$

We now summarize this as a theorem, and prove that the modified potential $\tilde{V}$ actually exists.

Theorem 3.5. The Newmark method with $\gamma = 1/2$ and any β, $0 \leqslant \beta \leqslant 1/2$ and h sufficiently small is the discrete Euler–Lagrange equations for the discrete Lagrangian L_{d}^{β} defined by

$$L_{\mathrm{d}}^{\beta}(q_0, q_1) = h\frac{1}{2}\left(\frac{\eta^\beta(q_1) - \eta^\beta(q_0)}{h}\right)^{\mathrm{T}} M\left(\frac{\eta^\beta(q_1) - \eta^\beta(q_0)}{h}\right) - h\tilde{V}(\eta^\beta(q_0)) \tag{28}$$

where $\eta^\beta(q_k) = q_k - h^2\beta M^{-1}\nabla V(q_k)$ and $\tilde{V}$ is defined so that $\nabla \tilde{V}(\eta^\beta(q_k)) = \nabla V(q_k)$ for all q_k.

Proof. If such a discrete Lagrangian is well defined then the above calculations show that the discrete Euler–Lagrange equations will give the Newmark algorithm with $\gamma = 1/2$ and the given β. We need only check that the modified potential function $\tilde{V}$ exists, given that it must satisfy the relation

$$\nabla \tilde{V}(\eta^\beta(q_k)) = \nabla V(q_k) \tag{29}$$

We introduce the following notation:

$$\begin{aligned} \eta^\beta(q) &= q - \beta h^2 M^{-1}\nabla V(q) \\ \xi^\beta(x) &= (\eta^\beta)^{-1}(x) \\ X(x) &= \nabla V(\xi^\beta(x)) \end{aligned}$$

and observe that we are trying to establish that $X(x)$ is the gradient of some function. A necessary and sufficient condition for this is for the following to hold:

$$\frac{\partial X_i}{\partial x^j} - \frac{\partial X_j}{\partial x^i} = 0 \quad \text{for all } i, j \tag{30}$$

Using $\nabla^2 V$ to denote the matrix of second partial derivatives of V and $D\xi^\beta$ to denote the matrix of derivatives of ξ^β we see that the left-hand side of (30) is

$$(\nabla^2 V D\xi^\beta)^{\mathrm{T}} - (\nabla^2 V D\xi^\beta) \tag{31}$$

Computing $D\eta^\beta = I - \beta h^2 M^{-1}\nabla^2 V$ it is clear that the symmetry of M and $\nabla^2 V$ implies that $D\eta^\beta$ satisfies the relation $(D\eta^\beta)^{\mathrm{T}}\nabla^2 V = \nabla^2 V\, D\eta^\beta$. Using the fact that $D\eta^\beta$ and $D\xi^\beta$ are inverses allows this to be rearranged to yield $\nabla^2 V\, D\xi^\beta = (D\xi^\beta)^{\mathrm{T}}\nabla^2 V$, and using again the symmetry of $\nabla^2 V$ shows that (31) is zero and thus condition (30) is satisfied.

Since we are working in $\mathbb{R}^n$, we conclude that a function $\tilde{V}$ with the desired property (29) exists, and so L_{d}^β is well defined and generates the Newmark method for $\gamma = 1/2$ and any β. □

3.5. Consequences of Newmark's variational nature

There are three ways of interpreting the variational and symplectic nature of the Newmark integrator. Firstly, one can consider the Newmark and variational schemes to be essentially the same, except the variational method has the right form to exactly conserve the momenta. As the two methods have almost identical implementations, one could simply change to using the variational integrator.

A second way to interpret this result is to realize that it implies that Newmark *will* exactly preserve momenta and a symplectic form, except they will not be quite the obvious ones we are used to writing down. It is possible to derive expressions for these momenta and the non-canonical symplectic form conserved by Newmark, but the expressions can be rather unwieldy. We give an example of this below. The observation of Simo *et al.* [1] that central differences Newmark preserves momenta evaluated at midpoints seems to be consistent with this.

Example. Let us work out the nature of the Newmark conserved quantity associated to the first co-ordinate being cyclic. We considered this example in the introduction for the variational algorithm. As usual, we consider a Lagrangian of the usual form of kinetic minus potential energy:

$$L(q, \dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}} M \dot{q} - V(q)$$

Assume that V is independent of the first component q^1 of q, so that $p_1 = [M\dot{q}]_1$ is a constant of the true continuous motion.

If we use the Newmark method to simulate this system, obtaining a trajectory $\{q_k\}$, then we know that the corresponding discrete momentum map derived from L_{d}^β will be conserved. Computing this gives

$$J_{\mathrm{d}} = \left[M \left(\frac{\eta^\beta(q_k) - \eta^\beta(q_{k-1})}{h} \right) D\eta^\beta(q_k) \right]_1$$

which will be a constant, that is, independent of k.

Note that η^{β} is the identity plus a term of order h^2. The naive approximation of p_1, using a simple finite difference approximation of $\dot{q}$, is thus related to the true discrete momentum by

$$J_{\mathrm{d}} = \left[M \left(\frac{q_k - q_{k-1}}{h} \right) \right]_1 + \mathcal{O}(h^2)$$

showing that the usual discretization of momentum will be preserved up to order h^2.

More useful than actually finding the exactly conserved structures is to use them in a third interpretation of the variational nature of Newmark. The existence of nearby conserved quantities allows us to conclude the following.

Theorem 3.6. For sufficiently small time-step h, a regular value of the momentum, and assuming that the solutions computed by the Newmark algorithm (22), (23) with $\gamma = 1/2$ are bounded for all time, then these solutions will have bounded momentum error, uniformly for all time, and this error will tend to zero as h tends to zero.

Proof. This follows from the fact that the corresponding exactly conserved quantity for the variational integrator will be evaluated at the interpolated shadowing points for the Newmark algorithm and that the algorithmic momentum level sets are uniformly close (in bounded regions) to the momentum level sets for h small. □

Using the correspondence between the Newmark and variational schemes, which are symplectic, we can also use results applicable to symplectic integrators to understand the behaviour of Newmark. An example of this is the work on the energy behaviour of symplectic integrators (see, for example, References [2, 36] and references therein).

Note that our results in no way guarantee stability of the Newmark method for *large time steps*. We have concentrated on a geometric analysis for nonlinear systems, and our results for structure preservation apply only for some (system dependent) bound on the timestep. As discussed in Hughes [34, 35], Newmark *can* perform badly on nonlinear systems with moderate timesteps. This is a reflection of the short time numerical stability behaviour of Newmark, rather than the geometric structure. In practice, of course, one must consider both the numerical accuracy and stability of an integration scheme, *as well as* its structure preserving qualities.

3.6. Minimization structure of the Newmark algorithm

In this section we consider a different way of writing the Newmark algorithm using optimization methods. This will be particularly useful when we come to algorithms for dissipative and forced systems, so we include forces in the formulation already here.

We consider a set of equations of motion of the form

$$M\ddot{q} + f^{\mathrm{int}}(q, \dot{q}) = f^{\mathrm{ext}}(t) \tag{32}$$

with $q(t) \in \mathbb{R}^n$, and where we regard $f^{\mathrm{ext}}(t)$ as a given external force. As for the internal force, we postulate the existence of a conservative potential $V(q)$ and a dissipative potential $\varphi(q, \dot{q})$ such that

$$f^{\mathrm{int}}(q, \dot{q}) = \frac{\partial V(q)}{\partial q} + \frac{\partial \varphi(q, \dot{q})}{\partial \dot{q}} \tag{33}$$

Dissipative potentials of this sort can be regarded as Rayleigh dissipation functions; we will discuss these in greater detail in the second half of this paper.

We discretize the equations of motion using the Newmark scheme as follows:

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}[(1-2\beta)a_k + 2\beta a_{k+1}] \tag{34}$$

$$Ma_{k+1} + f^{\text{int}}_{k+1} = f^{\text{ext}}_{k+1} \tag{35}$$

$$\dot{q}_{k+1} = \dot{q}_k + h[(1-\gamma)a_k + \gamma a_{k+1}] \tag{36}$$

We define

$$q^{\text{pre}}_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}[(1-2\beta)a_k]$$

so that (34) reads

$$q_{k+1} = q^{\text{pre}}_{k+1} + \beta h^2 a_{k+1}$$

To close this set of equations, we need to supply a relation between f^{int}_{k+1} and q_{k+1}. To this end, following Radovitzky and Ortiz [25], and Ortiz and Stainier [24], we introduce the *effective incremental potential*

$$V_k(q_{k+1}) = V(q_{k+1}) + h\varphi\left(q_{k+\sigma}, \frac{q_{k+1}-q_k}{h}\right) \tag{37}$$

where

$$q_{k+\sigma} = (1-\sigma)q_k + \sigma q_{k+1} \tag{38}$$

and $\sigma \in [0,1]$, and write

$$f^{\text{int}}_{k+1} = \frac{\partial V_k(q_{k+1})}{\partial q_{k+1}} \tag{39}$$

which is consistent with (33) as $h \to 0$ for any choice of σ.

The above algorithm can be recast in optimization form as follows. Combine (34) and (35) to get

$$M\frac{q_{k+1}-q^{\text{pre}}_{k+1}}{h^2} + \beta f^{\text{int}}_{k+1} = \beta f^{\text{ext}}_{k+1} \tag{40}$$

Clearly, this is the Euler–Lagrange equation of the function:

$$f(q_{k+1}) = \frac{1}{2h^2}(q_{k+1}-q^{\text{pre}}_{k+1})^{\text{T}} M(q_{k+1}-q^{\text{pre}}_{k+1}) + \beta V_k(q_{k+1}) - \beta f^{\text{ext}}_{k+1}\cdot q_{k+1} \tag{41}$$

Therefore, under appropriate convexity conditions on V and φ, the updated configuration follows as the solution of the minimum principle:

$$\min_{q_{k+1}} f(q_{k+1}) \tag{42}$$

Once q_{k+1} is determined, the internal forces are computed from Equation (39) and subsequently the velocities are updated using (36).

Some remarks about these results are in order:

1. The minimum principle for non-convex potentials can be replaced by a principle of stationarity. However, cases in which one has a minimum are useful to stress for they can be useful for error estimates and also for the use of optimization techniques, as in References [24, 28, 29].
2. The minimization principle operates on the *non-explicit* part of the Newmark algorithm. Thus, in this view, it can be regarded as a two-step procedure; first one computes the predictor point by an explicit formula and then, secondly, one corrects this with the minimization principle. This use of the term 'predictor' is special to this formulation. We shall use the term slightly differently in later sections.
3. Notice that in the case of conservative systems (so there are no external forces or dissipative potentials) this scheme is literally the Newmark scheme for conservative systems, which, as we have shown, is equivalent to a variational scheme. Thus, the same scheme has both a variational (and hence symplectic) interpretation as well as obeying an interesting minimization principle. These facts together should be useful in extending the analytical results on Newmark beyond what we have done.

4. NUMERICAL TESTS FOR CONSERVATIVE SYSTEMS

4.1. Example system

To illustrate the performance of some of the algorithms discussed in the preceding sections we consider a simple conservative system. The example chosen here is a two degree of freedom non-linear oscillator, consisting of a particle with unit mass moving in the plane with trajectory $q(t) \in \mathbb{R}^2$ under the influence of the potential

$$V(q) = \|q\|^2(\|q\|^2 - 1)^2$$

The Lagrangian describing this problem is thus

$$L(q, \dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}}\dot{q} - V(q)$$

and the equations of motion are the corresponding Euler–Lagrange equations.

Trajectories of this example system have two conserved quantities. First, the mechanical nature of the system implies that energy is conserved. Second, the fact that the potential V, and hence the Lagrangian L, is radially symmetric implies conservation of angular momentum.

We are interested here in the extent to which the different integration schemes actually preserve these two quantities. This is an issue related to, but different from, the absolute accuracy of trajectories. Although symplectic integration schemes frequently exhibit improved trajectory accuracy, this is not guaranteed. Nonetheless, we focus here on the preservation of invariants of the system since these properties will be reflected in an interesting way for the Newmark scheme.

4.2. Tested algorithms

The algorithms for which we present results here are:

- *Implicit Newmark*: Newmark with $\beta = 1/4,\ \gamma = 1/2$.
- *Explicit Newmark*: Newmark with $\beta = 0,\ \gamma = 1/2$.

- *Variational*: $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ variational integrator with $\alpha = 1/2$.
- *Runge–Kutta*: Fourth-order, fixed time-step.
- *Benchmark*: MATLAB 5.3 `ODE113` (predictor–corrector).

The fourth-order Runge–Kutta method is a classical integrator which makes no use of the mechanical nature of the system. It is included to demonstrate the behaviour which occurs if one treats the system as an arbitrary set of equations, rather than taking advantage of their mechanical structure.

All the integrators except for the benchmark code are run with the same step size of $h = 0.2$ to provide a reasonable comparison between them. The benchmark code is a high-order, multi-step, predictor–corrector method which we run with a very small step size. On an example this simple, the benchmark method can be regarded as essentially identical to the true solution.

The energy at each time-step is evaluated as the energy on TQ. That is, for the variational method we use the pull-back of the true energy under the discrete fibre derivative.

4.3. Results

The energy behaviour of the various integrators is shown for a short time in Figure 2. The same pattern is observed if the simulation is carried out for essentially arbitrarily long times. It is immediately apparent from this figure that the Newmark and variational methods have qualitatively different behaviour to the Runge–Kutta technique. This fluctuating energy behaviour of variational schemes is typical of symplectic methods, and provides a clear indication that Newmark is in fact symplectic.

The evolution of the angular momentum with the various integrators is plotted in Figure 3. The results for the variational algorithm and the explicit Newmark method are not shown, because they exactly conserve the angular momentum of the system, as explained previously. In this figure we see clearly the Newmark behaviour implied by Theorem 3.6 and that result shows that this oscillatory behaviour will persist *indefinitely*. While a standard integrator will have divergent momentum behaviour, the fact that Newmark in variational under a near-identity change of co-ordinates forces the angular momentum to be almost conserved, with at most the finite fluctuations seen here.

We must caution against attempts to interpret the variations in energy as percentage or relative errors. This is because the energy of the system is only meaningful up to an additive constant and so the initial energy, or energy at any given time, is entirely arbitrary. It is also not significant that the energies of the various trajectories all lie either above or below the exact value. This is due to the simple nature of the example system, and is not apparent for more complex problems.

Note that the accuracy of the benchmark algorithm is demonstrated by the fact that it preserves the energy and momentum to within almost machine precision. This will be of use when we perform numerical tests on dissipative systems for which the true behaviour cannot be analytically calculated.

5. NUMERICAL ALGORITHMS FOR SYSTEMS WITH FRICTION

Now we consider non-conservative systems; those with forcing and in particular, those with dissipation. The dissipation considered here is of simple Rayleigh dissipation type. In other publications [29] we use these methods in collision problems with Coulomb friction.

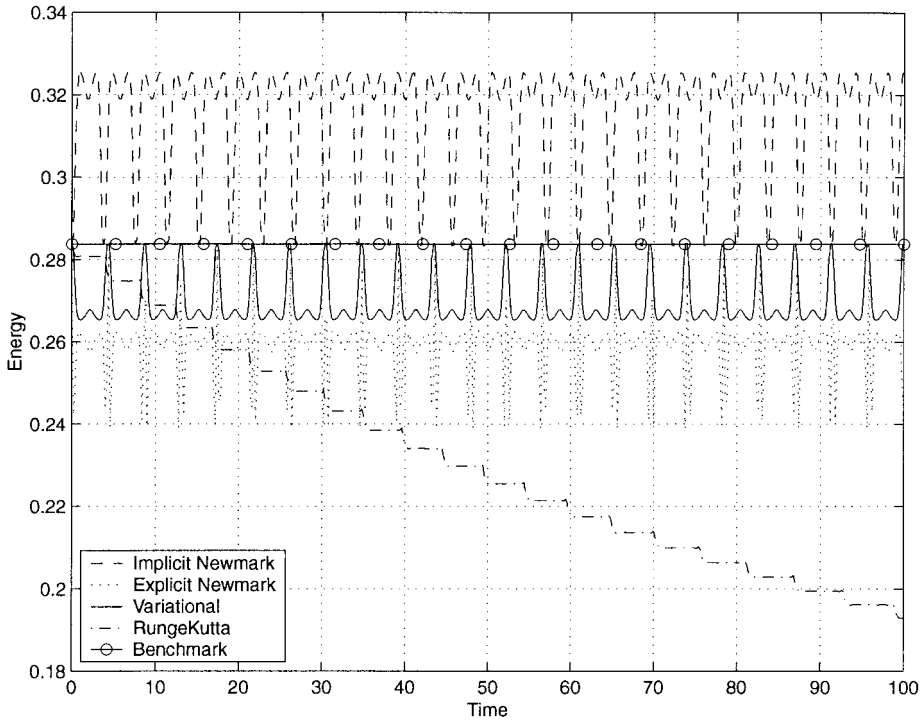

Figure 2. Energy behaviour of integrators for a conservative system. Note the long-time stable behaviour typical of the variational method, as contrasted to classical methods such as Runge–Kutta. The stable behaviour of Newmark is explained by its variational nature.

We consider a given Lagrangian $L(q, \dot{q})$ and associated dissipative systems with Rayleigh-type dissipation of the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = -\frac{\partial \varphi}{\partial \dot{q}}(q, \dot{q})$$

where $\varphi(q, \dot{q})$ is a given dissipative potential. We are specifically interested in the case when L has the form

$$L(q, \dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}} M \dot{q} - V(q)$$

where $q \in \mathbb{R}^n$, M is a constant mass matrix (a positive-definite symmetric $n \times n$ matrix) and V is a given potential energy function, so that the equations take the form

$$M\ddot{q} = -\nabla V(q) - \frac{\partial \varphi}{\partial \dot{q}}(q, \dot{q})$$

Let the energy be denoted

$$E(q, \dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}} M \dot{q} + V(q)$$

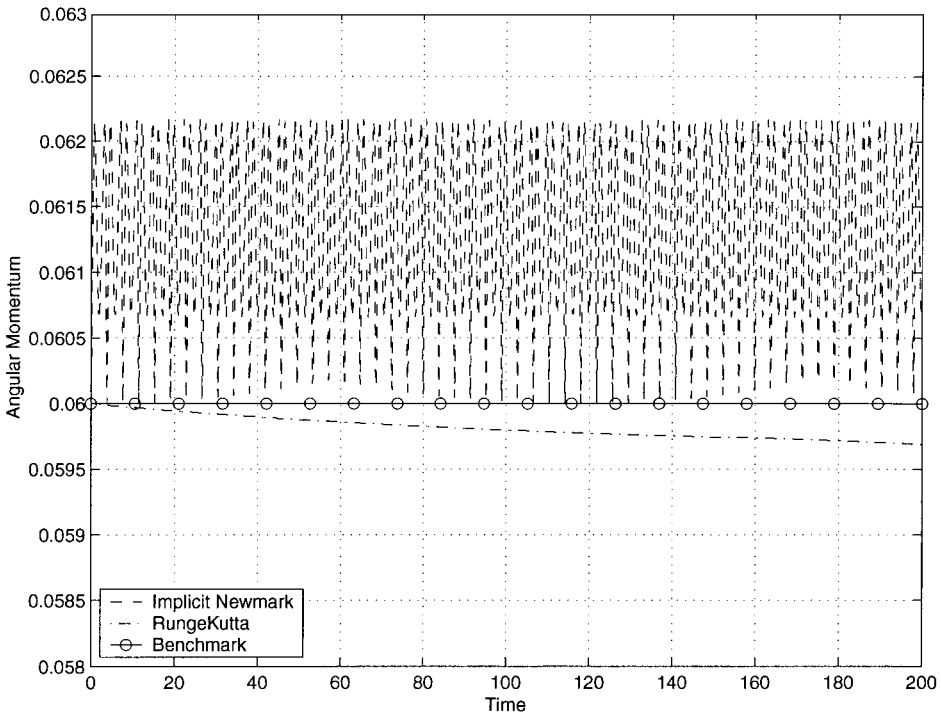

Figure 3. Momentum behaviour of integrators for a conservative system. Variational results are not plotted as they exactly conserve momenta. Note the predicted long-time stable behaviour of Newmark, as contrasted against the divergent behaviour of methods such as Runge–Kutta.

and recall the usual energy equation

$$\frac{\mathrm{d}}{\mathrm{d}t}E = -\left\langle \dot{q}, \frac{\partial \varphi}{\partial \dot{q}}(q,\dot{q}) \right\rangle$$

The standard example is of course the case

$$\varphi(q,\dot{q}) = \tfrac{1}{2}\dot{q}^{\mathrm{T}} R \dot{q}$$

where R is a positive-definite symmetric matrix, so that the energy equation becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}E = -\dot{q}^{\mathrm{T}} R \dot{q} \leqslant 0$$

Our aim is to develop algorithms that have good energy decay properties in the sense that the algorithms predict the correct energy drop after a long integration run. We shall consider three types of algorithms (not necessarily in order of performance or preference):

1. Algorithms based on a discretization of the Lagrange–d'Alembert principle as a generalization of variational integrators.
2. Two step integration methods that separate the algorithms into conservative and dissipative parts.

3. Minimization algorithms that are directly related to the Newmark algorithm with forces. Here the steps are based on explicit–implicit splits.

We will consider these in turn.

5.1. Discrete Lagrange–d'Alembert principle

Recall that the (continuous) *integral Lagrange–d'Alembert principle* is

$$\delta \int L(q(t), \dot{q}(t))\,\mathrm{d}t + \int F(q(t), \dot{q}(t)) \cdot \delta q\,\mathrm{d}t = 0 \tag{43}$$

We define the *discrete Lagrange–d'Alembert principle* to be

$$\delta \sum L_{\mathrm{d}}(q_k, q_{k+1}) + \sum [F_{\mathrm{d}}^{-}(q_k, q_{k+1}) \cdot \delta q_k + F_{\mathrm{d}}^{+}(q_k, q_{k+1}) \cdot \delta q_{k+1}] = 0 \tag{44}$$

where L_{d} is the discrete Lagrangian and F_{d}^{-} and F_{d}^{+} are the left and right discrete forces.

Equation (44) defines an integrator $(q_k, q_{k+1}) \mapsto (q_{k+1}, q_{k+2})$ given implicitly by the *forced discrete Euler–Lagrange equations*:

$$D_1 L_{\mathrm{d}}(q_{k+1}, q_{k+2}) + D_2 L_{\mathrm{d}}(q_k, q_{k+1}) + F_{\mathrm{d}}^{-}(q_{k+1}, q_{k+2}) + F_{\mathrm{d}}^{+}(q_k, q_{k+1}) = 0 \tag{45}$$

Example. The discrete force analogues of the symmetric discrete Lagrangian $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$ given in Equation (16) are

$$F_{\mathrm{d}}^{\mathrm{sym},\alpha-}(q_0, q_1) \cdot \delta q_0 = h\frac{1}{2}\left[(1-\alpha)F\left(q_{0+\alpha}, \frac{q_1 - q_0}{h}\right) + \alpha F\left(q_{1-\alpha}, \frac{q_1 - q_0}{h}\right)\right] \cdot \delta q_0$$

$$F_{\mathrm{d}}^{\mathrm{sym},\alpha+}(q_0, q_1) \cdot \delta q_1 = h\frac{1}{2}\left[\alpha F\left(q_{0+\alpha}, \frac{q_1 - q_0}{h}\right) + (1-\alpha)F\left(q_{1-\alpha}, \frac{q_1 - q_0}{h}\right)\right] \cdot \delta q_1$$

where the interpolated positions are $q_{k+\alpha} = (1-\alpha)q_k + \alpha q_{k+1}$.

With these discrete forces and the discrete Lagrangian given by $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$, the forced discrete Euler–Lagrange equations (45) define a second-order accurate integrator for arbitrary Lagrangian L and arbitrary force F. In the particular case of $L = (1/2)\dot{q}^{\mathrm{T}} M \dot{q} - V(q)$ and $F = F(\dot{q})$ the integrator has the special form

$$\frac{1}{h}(-q_{k+2} + 2q_{k+1} - q_k) + \frac{h}{2}(1-\alpha)a_{k+1+\alpha} + \frac{h}{2}\alpha a_{k+2-\alpha} + \frac{h}{2}\alpha a_{k+\alpha} + \frac{h}{2}(1-\alpha)a_{k+1-\alpha}$$
$$+ \frac{h}{2}F\left(\frac{q_{k+2} - q_{k+1}}{h}\right) + \frac{h}{2}F\left(\frac{q_{k+1} - q_k}{h}\right) = 0 \tag{46}$$

Some numerics and tests of this variational Lagrange–d'Alembert method are given below. □

5.2. The Newmark algorithm with forcing is variational

It is interesting to note that for forces linear in $\dot{q}$, such as linear viscous friction, the techniques used to show that Newmark trajectories are shadowed by variational trajectories still apply, at least

for the case $\beta = 1/4$ and $\gamma = 1/2$. That is, trajectories of the average acceleration Newmark with a linear viscous term added by setting $a_k = M^{-1}[-\nabla V(q_k) - \gamma \dot{q}]$ are shadowed, in the precise sense, by trajectories of the variational Lagrange–d'Alembert inegrator (46) with $F(\dot{q}) = -\gamma \dot{q}$.

Considerably greater insight may be achieved, however, by the realization that the technique of Suris used in Section 3.4 can be extended to the forced case by the appropriate choice of discrete force functions, showing that Newmark with forcing is indeed a variational algorithm in the sense of the discrete Lagrange–d'Alembert principle.

The Newmark algorithm for a mechanical system with external forces $F(q, \dot{q})$ is given by

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}[(1 - 2\beta)a_k + 2\beta a_{k+1}] \tag{47}$$

$$\dot{q}_{k+1} = \dot{q}_k + h[(1 - \gamma)a_k + \gamma a_{k+1}] \tag{48}$$

where we now include forces in the acceleration terms to give

$$a_k = M^{-1}[-\nabla V(q_k) + F(q_k, \dot{q}_k)] \tag{49}$$

The implicit function theorem can be used to check that (for h sufficiently small) the Newmark equations (47)–(49) implicitly define a mapping $(q_k, q_{k+1}) \mapsto (\dot{q}_k, \dot{q}_{k+1})$. This allows us to replace the force evaluations in (49) with the expressions $F_{\mathrm{NM}}^{\beta-}$ and $F_{\mathrm{NM}}^{\beta+}$ defined by

$$F_{\mathrm{NM}}^{\beta-}(q_k, q_{k+1}) = F(q_k, \dot{q}_k) \tag{50}$$

$$F_{\mathrm{NM}}^{\beta+}(q_k, q_{k+1}) = F(q_{k+1}, \dot{q}_{k+1}) \tag{51}$$

where $\dot{q}_k$ and $\dot{q}_{k+1}$ are given by the implicit mapping defined by the Newmark equations.

Having made this force substitution now allows us to write Newmark with forcing as an update of configuration points, in the same way as Section 3.1. This yields

$$\begin{aligned}
&\frac{1}{h}(q_{k+2} - 2q_{k+1} + q_k) \\
&\quad + \beta h M^{-1} \nabla V(q_{k+2}) - (2\beta - 1) h M^{-1} \nabla V(q_{k+1}) + \beta h M^{-1} \nabla V(q_k) \\
&\quad - \beta h M^{-1} F_{\mathrm{NM}}^{\beta+}(q_{k+1}, q_{k+2}) + \frac{1}{2}(2\beta - 1) h M^{-1} F_{\mathrm{NM}}^{\beta-}(q_{k+1}, q_{k+2}) \\
&\quad + \frac{1}{2}(2\beta - 1) h M^{-1} F_{\mathrm{NM}}^{\beta+}(q_k, q_{k+1}) - \beta h M^{-1} F_{\mathrm{NM}}^{\beta-}(q_k, q_{k+1}) = 0
\end{aligned} \tag{52}$$

We will now establish that this algorithm can be derived as the forced discrete Lagrange–d'Alembert equations for the appropriate choice of discrete Lagrangian and discrete forces.

Theorem 5.1. The Newmark method with $\gamma = 1/2$ and any β acting on a forced system is, for sufficiently small h, the forced discrete Euler–Lagrange equations for the discrete Lagrangian L_{d}^{β}

and discrete forces $F_{\mathrm{d}}^{\beta-}$ and $F_{\mathrm{d}}^{\beta+}$ defined by

$$L_{\mathrm{d}}^{\beta}(q_0,q_1)=h\frac{1}{2}\left(\frac{\eta^{\beta}(q_1)-\eta^{\beta}(q_0)}{h}\right)^{\mathrm{T}}M\left(\frac{\eta^{\beta}(q_1)-\eta^{\beta}(q_0)}{h}\right)-h\tilde{V}(\eta^{\beta}(q_0)) \tag{53}$$

$$F_{\mathrm{d}}^{\beta-}(q_0,q_1)=h\frac{1}{2}[(1-2\beta)F_{\mathrm{NM}}^{\beta-}(q_0,q_1)+2\beta F_{\mathrm{NM}}^{\beta+}(q_0,q_1)]D\eta^{\beta}(q_0) \tag{54}$$

$$F_{\mathrm{d}}^{\beta+}(q_0,q_1)=h\frac{1}{2}[2\beta F_{\mathrm{NM}}^{\beta-}(q_0,q_1)+(1-2\beta)F_{\mathrm{NM}}^{\beta+}(q_0,q_1)]D\eta^{\beta}(q_1) \tag{55}$$

where $\eta^{\beta}(q_k)=q_k-h^2\beta M^{-1}\nabla V(q_k)$, $\tilde{V}$ is defined so that $\nabla\tilde{V}(\eta^{\beta}(q_k))=\nabla V(q_k)$ for all q_k and the functions $F_{\mathrm{NM}}^{\beta-}$ and $F_{\mathrm{NM}}^{\beta+}$ are as defined in (50) and (51).

Proof. We begin by noting that the discrete Lagrangian L_{d}^{β}, the mapping η^{β} and the modified potential $\tilde{V}$ are all identical to those used in Theorem 3.5 for the unforced conservative case. We therefore know that $\tilde{V}$ and thus L_{d}^{β} are well defined, and we have already established above that $F_{\mathrm{NM}}^{\beta-}$ and $F_{\mathrm{NM}}^{\beta+}$ exist, and hence so do $F_{\mathrm{d}}^{\beta-}$ and $F_{\mathrm{d}}^{\beta+}$. It only remains to check that the forced discrete Euler–Lagrange equations for (53)–(55) give the position-update form (51) of forced Newmark.

This is a simple matter of evaluating (45), multiplying on the right by the inverse of $D\eta^{\beta}(q_1)$ and substituting the expression for η^{β}. Rearranging then immediately gives (51), as claimed. □

The fact that Newmark with $\gamma=1/2$ is a second-order accurate discrete Lagrange–d'Alembert integrator implies that its performance should be similar to that of the algorithm (46). As we will see in the numerical tests in Section 6, this is indeed the case.

5.3. A two-step variational principle for friction

Next, we explore a two step algorithm for problems with friction where the two steps are designed to split the algorithm into conservative and dissipative parts. We will stick with the case of a Lagrangian of the form kinetic minus potential energies for simplicity. The second step is based on an interesting minimization principle.

We believe this algorithm and its companion algorithm which uses an explicit–implicit split, which are based on optimization methods, may be useful in certain large problems where the computational savings using optimization techniques can be employed. However, in the present paper we consider only simple, low-dimensional numerical examples. These two step algorithms are employed in the work on collisions (see References [28, 29]).

Given (q_0,q_1), we first compute the point q_2^{pred} according to the discrete Euler–Lagrange equations for a given L_{d}. For example, with the discrete Lagrangian L_{d}^{α} with $\alpha=1/2$, q_2^{pred} satisfies

$$M\left[\left(\frac{q_2^{\mathrm{pred}}-2q_1+q_0}{h^2}\right)\right]+\frac{1}{2}\left[V'\left(\frac{q_0+q_1}{2}\right)+V'\left(\frac{q_1+q_2^{\mathrm{pred}}}{2}\right)\right]=0 \tag{56}$$

Of course, as we showed in the first part of the paper, suitably interpreted, this step also includes the Newmark algorithm. Then we follow this with a second (dissipative) step, which consists of minimizing the discrete kinetic energy plus the dissipative potential with respect to the *last endpoint*.

That is, we extremize the following expression with respect to the *final* endpoint q_2:

$$\frac{1}{2}\left(\frac{q_2 - q_2^{\text{pred}}}{h}\right)^{\mathrm{T}} M\left(\frac{q_2 - q_2^{\text{pred}}}{h}\right) + h\varphi\left(\frac{q_2 - q_1}{h}\right) \tag{57}$$

In other words, the equation satisfied by q_2 is given by

$$M\left(\frac{q_2 - q_2^{\text{pred}}}{h^2}\right) + \varphi'\left(\frac{q_2 - q_1}{h}\right) = 0 \tag{58}$$

Adding (56) and (58), we see that the term involving q_2^{pred} cancels and we get

$$M\left[\left(\frac{q_2 - 2q_1 + q_0}{h^2}\right)\right] + \frac{1}{2}\left[V'\left(\frac{q_0 + q_1}{2}\right) + V'\left(\frac{q_1 + q_2^{\text{pred}}}{2}\right)\right] + \varphi'\left(\frac{q_2 - q_1}{h}\right) = 0 \tag{59}$$

which is consistent with the original equations.

We summarize the result in the following

Theorem 5.2. For a Lagrangian of the form kinetic minus potential energy, the following two-step algorithm is consistent with the equations of motion with dissipative forces derived from a dissipative potential φ:

Step 1: Map (q_{n-1}, q_n) to $(q_n, q_{n+1}^{\text{pred}})$ by means of the discrete Euler–Lagrange equations for a choice of discrete Lagrangian L_{d}.

Step 2: Map $(q_n, q_{n+1}^{\text{pred}})$ to (q_n, q_{n+1}) by extremizing

$$K_{\text{d}}(q_{n+1}, q_{n+1}^{\text{pred}}) + h\varphi\left(\frac{q_{n+1} - q_n}{h}\right)$$

where K_{d} is the discrete kinetic energy, with respect to the final endpoint q_{n+1}.

While this algorithm is not literally a product formula (in the sense of, e.g., Reference [34]), it has some of the same spirit. It would be of interest of course to see to what extent one can prove things about the behaviour of the symplectic form and the energy.

5.4. Minimization structure of Newmark with friction

As we explained in Section 3.6, one can write the Newmark algorithm with external forces using an explicit–implicit split, where all of the implicit part of the algorithm is bundled with a minimization step. We just note that compared to other possible formulations of Newmark, the minimization scheme has an additional parameter σ used for interpolation in the force evaluations, so it may depart slightly from other Newmark schemes with external forcing. In the Newmark simulations below, we mean the ones generated by the scheme given in Section 3.6 with the computed acceleration initialized to the true acceleration.

One of the advantages of the optimization approach in the scheme here as well as the one in the preceding section is that it extends in a natural way to problems with Coulomb friction, where one has to also do an optimization over the friction cone; however, the basic structure of the scheme remains intact. As we have remarked, this extension of the present method combined with our work on collisions is discussed in Reference [29].

6. NUMERICAL TESTS FOR DISSIPATIVE SYSTEMS

6.1. Example system

To demonstrate the behaviour of the algorithms developed in the previous section we consider the same non-linear oscillator used in Section 4 with a small amount of linear viscous dissipation. In the notation used in the previous section, we use the dissipative potential given by

$$\varphi(\dot{q}) = \frac{10^{-3}}{2}\dot{q}^{\mathrm{T}}\dot{q}$$

which corresponds to a force of

$$F(\dot{q}) = -10^{-3}\dot{q}$$

We have chosen a weakly dissipative system to highlight the advantages of the Newmark, variational and two-step methods. If the dissipation is too high, then all trajectories quickly decay to zero energy and it is difficult to distinguish any differences between the integrators.

As for the conservative example presented previously, we concentrate here on the accuracy of the integrators at estimating the energy and momentum evolution. The dissipative nature of the system implies that both quantities should decrease, so the test becomes the correct estimation of the overall decay of energy and momentum.

6.2. Tested algorithms

We present results for the same methods used on the conservative system, except that here we use the two extensions to the variational algorithm for dissipative systems, namely the discrete Lagrange–d'Alembert method and the two-step minimum work method:

- *Implicit Newmark*: Newmark with $\beta = 1/4$, $\gamma = 1/2$.
- *Explicit Newmark*: Newmark with $\beta = 0$, $\gamma = 1/2$.
- *Variational*: $L_{\mathrm{d}}^{\mathrm{sym},\alpha}$, $F_{\mathrm{d}}^{\mathrm{sym},\alpha}$ discrete Lagrange–d'Alembert method with $\alpha = 1/2$.
- *Two-step*: Two-step minimum work method.
- *Runge–Kutta*: Fourth-order, fixed time-step.
- *Benchmark*: MATLAB 5.3 `ODE113` (predictor–corrector).

The integration parameters, such as step size and method of energy evaluation, are all identical to those used in Section 4 for the numerical tests in the conservative case.

6.3. Results

Two tests are presented here, both on the same system. In Figure 4 the simulation is run for the same time length as was the conservative system in Section 4. As a more dramatic demonstration we also run the system for a very much longer time, as given in Figure 5. In both cases we plot only the energy decay. We do not give the corresponding momentum plots, as they are qualitatively similar to the energy.

For the example system, the discrete Lagrange–d'Alembert variational method and the two-step variational method give results which are almost indistinguishable. For this reason only a single 'Variational' trajectory is plotted in Figures 4 and 5. This should be taken as representative of

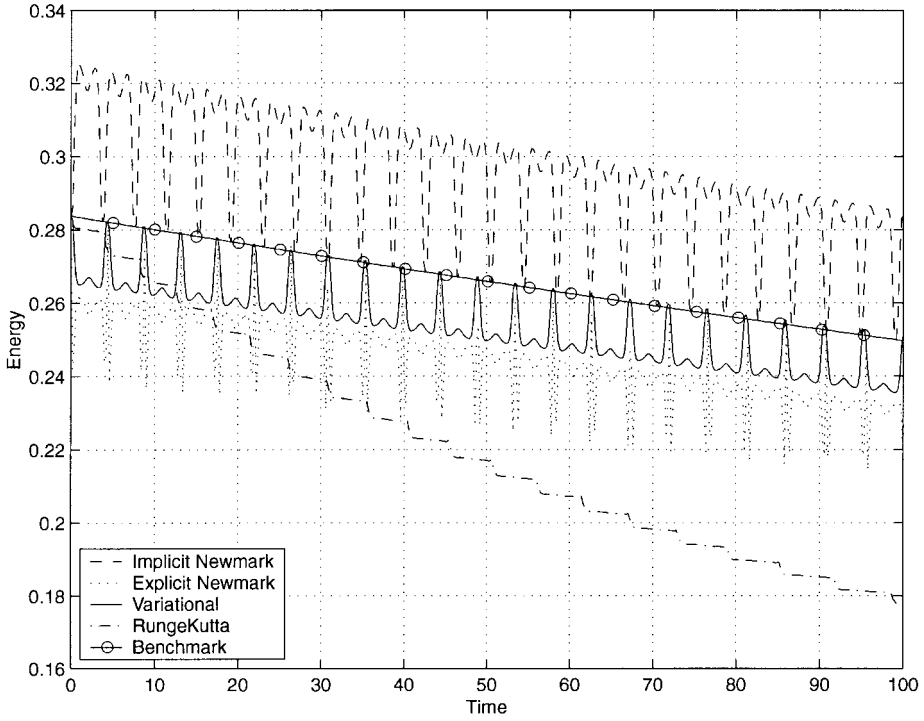

Figure 4. Energy behaviour of integrators for a dissipative system. The variational integrators accurately simulate energy decay, unlike standard methods such as Runge–Kutta.

both the discrete Lagrange–d'Alembert variational method and the two-step variational method. The crucial aspect of both of these algorithms is their variational nature.

From these results it is clear that the Newmark method, the discrete Lagrange–d'Alembert method and the two-step minimum work method all correctly capture the energy decay, unlike traditional methods such as Runge–Kutta. When the simulation is continued for longer times, this good behaviour continues, although there are slight deviations at very large times.

The particularly impressive aspect of the energy decay predictions of the variational integrators is that they are only low-order methods, unlike the fourth-order accurate Runge–Kutta. This is a clear demonstration of the fact that traditional measures of integrator accuracy, such as local truncation error, are not necessarily appropriate when discussing variational or symplectic schemes, as they often perform far better than expected.

As shown previously, the Newmark algorithm is variational, and so we expect the good energy behaviour seen here. For this reason we have omitted the Newmark method from the longer time simulation, in order to make the results clearer. In that case Newmark performs similarly to the other variational methods.

The variational integrators for dissipative systems are expected to be particularly useful for systems which are nearly conservative, such as mechanical systems with weak dissipation or weak forcing. This is due to the fact that they perform very well on the main conservative part of the system, the area where traditional integration schemes introduce most of the error.

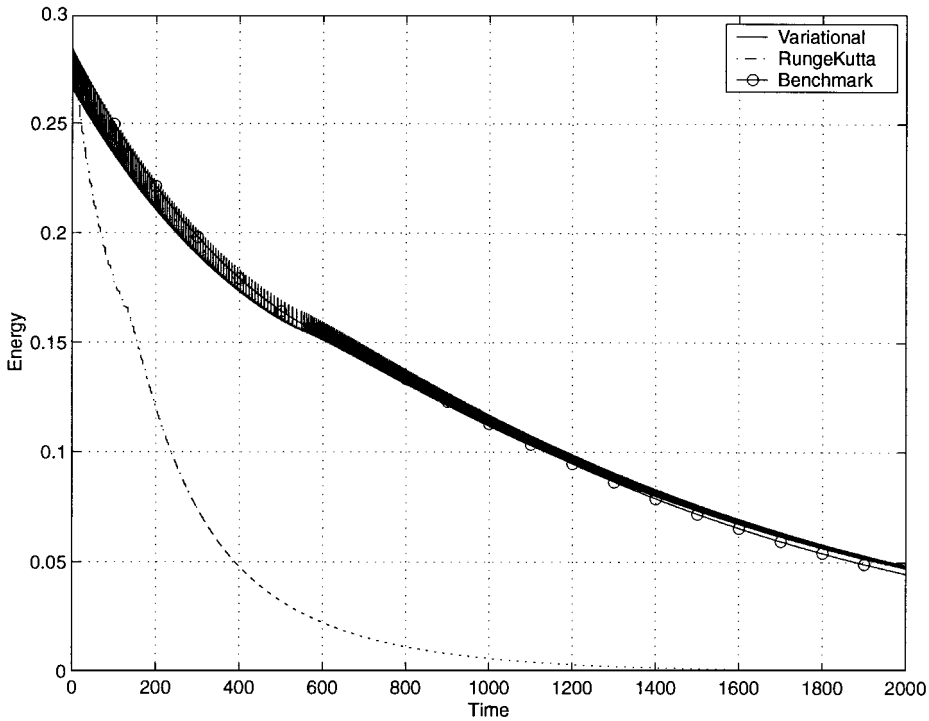

Figure 5. Energy behaviour of integrators for a dissipative system. The variational integrators accurately simulate energy decay, unlike standard methods such as Runge–Kutta.

Although the example chosen here is very simple, it captures the important aspects of the numerical behaviour of the variational algorithms. The performance of the algorithms on high degree of freedom systems, such as finite element discretizations, is of considerable interest.

7. CONCLUSIONS AND FUTURE WORK

We conclude with some general comments and possible directions for future work.

Higher-order integrators: In future work we plan to develop higher-order integrators based on, for example, more accurate approximations to the action integral. This is closely related to the technique of forming good approximations to the Hamilton–Jacobi equation, as in Reference [38], but we believe that one can sometimes be better off using Jacobi's solution to the Hamilton–Jacobi equation (the integral of the Lagrangian along a solution to the Euler–Lagrange equations) and approximating this integral.

Non-linear analysis of Newmark: It is quite possible that the techniques of this paper can be used to give a non-linear analysis showing the good long-time performance of the Newmark algorithm. At the moment, most of the analysis is that of error analysis type and for linear systems.

Time adaptive algorithms: As shown in Reference [6], one can achieve conservation of energy in addition to conserving the symplectic structure (in an appropriate spacetime sense) and momentum

by using time adaptive techniques. It would be of interest to explore the numerical implications of this further in the context of the present paper.

Collisions: In Reference [29] algorithms for collision problems are developed. In fact, those algorithms are consistent with those presented in this paper. The paper [17] explores the addition of friction to these algorithms.

Multisymplectic integrators: Another area of interest is the development of multisymplectic integrators for PDE's following Marsden *et al.* [5]. It would be of interest to explore these integrators using Newmark methods coupled with finite element techniques as well as with the addition of friction or forcing.

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