Variational Integrators and the Newmark algorithm

ME 6106 Computational Structural Dynamics - Course Project

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Abstract

The aim of this article is to review the variational approach to Mechanics and Mechanical integrators, and show how the Newmark family of integrators are variational in a certain sense. This variational nature is believed to be the primary reason why this class of algorithms perform so well, and are so very widely used, especially in the structural dynamics community.

The theory of Variational Integrators is a very active area of research, and has been utilized to solve a wide variety of problems in Mechanical and Aerospace Engineering. It is well known that variational integrators preserve certain invariants of the original continuous time system, such as energy and momentum. A consequence of this is that variational integrators exhibit excellent energy behaviour over long periods of integration, unlike other classical integration schemes such as Runge Kutta methods. The fact that the Newmark family of integration algorithms are variational implies that they inherit these preservation properties.

We shall show in this article what exactly it means for an integration scheme to be variational. We show that the Newmark family of integrators satisfy this criteria, and so is variational in nature. We also validate through simulations our prediction that this class of algorithms preserve certain invariants like energy and momentum of the original system, in the case of a conservative mechanical system with 100,000 degrees of freedom.

Contents

Chapter 1

Introduction

This article has two main objectives. First, we review the theory of discrete Lagrangian mechanics and the construction of variational integrators. Second, we show that the Newmark scheme, which is widely used widely in structural dynamics is variational in nature, and we explore and validate some consequences of this fact through numerical simulations. The article mainly follows the contents of the paper [KMOW00], although some extra material has been added from various sources to make the article more readable.

The fundamental idea behind variational integrators is that the motion of mechanical systems can be described using Hamilton's principle of least action; the path taken by a mechanical system between times 0 and T and configuration q_0 and q_1 is the one for which the integral of the Lagrangian is stationary to first order (we will make the meanings of these terms more precise in the following sections). Traditionally, time integration algorithms for mechanical systems were constructed by discretizing the ordinary differential equations which describe the motion of a system to give difference equation which were then solved to give a discrete trajectory. Such algorithms are oblivious to the fact that for mechanical systems, the ODEs describing the equations of motion are arrived at by finding necessary conditions for a trajectory to be a stationary point of the integral of the Lagrangian. Because of this, classical time integration algorithms could not exploit the fact that symmetries in the Lagrangian lead to invariants of the flow of the system. Variational integrators exploit the Hamilton's principle of least action. Instead of directly discretizing the ODEs to give difference equations, the action integral is discretized to give an action sum corresponding to a discrete trajectory, and the stationary trajectories of the action sum is treated as the approximation of the continuous time trajectory. To arrive at an action sum, typically we first arrive at a discrete Lagrangian. To construct integrators which preserve invariants of the flow, it is simply enough to construct discrete Lagrangian which inherit the symmetries of the continuous Lagrangian.

The theory of Variational integrators is not limited to the integration of mechanical systems, a non-exhaustive list of applications include: integration of bodies undergoing collision [FMOW03], optimal control of mechanical systems [OBJM11], medical image analysis [MM07]. Also, in this article, we only consider finite dimensional mechanical systems. But variational integrators have been extended to solve infinite dimensional problems, such as in Fluid mechanics [MS99].

The Newmark family of methods, first proposed in [New59], is a very popular time integration algorithm in the structural dynamics community. It has been observed that the Newmark methods have remarkable near energy preserving properties, often better than that of higher order schemes for moderately long time integration. It is the author's belief that the variational nature of the Newmark family is an important reason why this is so.

The article is organized as follows. Chapter 2 is a review of continuous time Lagrangian mechanics. We introduce standard concepts from Lagrangian mechanics such as the action integral, Euler Lagrange equations, fiber derivative and the Lagrangian symplectic form. In Chapter 3, we introduce discrete Lagrangian mechanics. We define concepts corresponding to those from continuous time Lagrangian mechanics. In chapter 4, we introduce variational integrators. We show how variational integrators preserves a certain symplectic form and energy. In chapter 5, we introduce the Newmark family of time integration algorithms and we show that these are indeed variational in nature. In chapter 6, we compare the energy behaviour of some integrators from the Newmark family with Runge Kutta method of order 4, and Matlab's ode45 through simulations. In chapter 7, the article is concluded with some final remarks.

Chapter 2

Continuous Lagrangian Mechanics

2.1 Basic Definitions

We consider a mechanical system evolving on the configuration space $Q = \mathbb{R}^n$ with associated state space given by $TQ = T\mathbb{R}^n = \mathbb{R}^n \times \mathbb{R}^n$. The state space is just the collection of ordered pairs of generalized positions and velocities, the first element of the pair being position and the latter velocity. Similarly, the phase space of the system is given by $T^*Q = T^*\mathbb{R}^n = \mathbb{R}^n \times (\mathbb{R}^n)^*$, where $(\mathbb{R}^n)^*$ is the dual space of $\mathbb{R}^n$, the set of covectors of $\mathbb{R}^n$. The phase space can be thought of as the set of ordered pairs of generalized positions and momenta. Momentum is treated as a covector because momentum acts on velocity linearly to give a real number, the kinetic energy scaled by a factor of two. Let $K : TQ \mapsto \mathbb{R}$ and $V : Q \mapsto \mathbb{R}$ denote the Kinetic and Potential energy of the system respectively. We define the Lagrangian $L : TQ \mapsto \mathbb{R}$ to be

$$L(q, \dot{q}) = K(q, \dot{q}) - V(q)$$

We assume the Lagrangian is C^2 smooth throughout the article. Given an interval $[0, T]$, we define the path space to be

$$C(Q) = \{q : [0, T] \mapsto Q |\ q \text{ is a } C^2 \text{ curve}\}$$

and the action map $S : C(Q) \mapsto \mathbb{R}$ to be

$$S(q) = \int_0^T L(q(t), \dot{q}(t)) dt.$$

Theorem 1 (Hamilton's principle of least action). *A mechanical system moves from configuration q_0 to q_1 between time* 0 *to* T *along the curve* $q \in C(Q)$ *which satisfies*

$$\delta S(q)[\delta q] = 0 \tag{2.1}$$

for all variations δq of q with endpoints fixed at q_0 and q_1. We shall call this curve the Euler-Lagrange curve between points q_0 and q_1. It is well know that the condition 2.1 is equivalent to

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0 \tag{2.2}$$

along the curve q.

In the above theorem, it is assumed that the reader is familiar with the variation of a functional. We refer the reader to [HSS09] for more details and a proof of the above theorem.

Equation 2.2 is called the Continuous time Euler Lagrange (EL) equation. Under some regularity assumptions on L, it is a second order ordinary differential equation which gives the equations of motion of a mechanical system.

We shall denote the flow generated by the Euler Lagrange equations by $F_L^T : TQ \mapsto Q$. $F_L^T(q_0, \dot{q}_0)$ just gives the point on the configuration space that a system which at time $t = 0$ is at position q_0 with velocity $\dot{q}_0$ reaches at time $t = T$.

We define the Fiber derivative $\mathbb{F}L : TQ \mapsto T^*Q$ to be

$$\mathbb{F}L(q, \dot{q}) = (q, \frac{\partial L}{\partial \dot{q}}(q, \dot{q})) \tag{2.3}$$

Remark 1. It is to be noted that the Fiber derivative is just the Legendre transform of L. There is another viewpoint to Classical mechanics; Hamiltonian mechanics. Hamiltonian mechanics describes the motion of a mechanical system on the phase space, as opposed to the state space in Lagrangian mechanics. The Fiber derivative acts as a bridge between Lagrangian and Hamiltonian mechanics. For most concepts defined in Lagrangian mechanics, there exists a counterpart in Hamiltonian mechanics, and more often than not, the Fiber derivative is used in some form to connect the two. Throughout this article, we will only focus on the Lagrangian viewpoint.

Example 1 (Mass-Spring system)**.** Let the Lagrangian be

$$L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M\dot{q} - \frac{1}{2}q^T Kq$$

where $M = M^T \succ 0, K = K^T \succeq 0$. Then, the Euler Lagrange equations are

$$M\ddot{q} + Kq = 0.$$

This is the well known equations of motion of a Mass-Spring system. The Fiber derivative is given by

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

We see that in this case, the Fiber derivative is just the linear momentum of the system.

2.2 Invariants of the Flow

2.2.1 Lagrangian Energy

We define the energy associated with the Lagrangian L to be $E : TQ \mapsto \mathbb{R}$ given by

$$E(q,\dot{q}) = \frac{\partial L}{\partial \dot{q}}\dot{q} - L(q,\dot{q}) \tag{2.4}$$

Theorem 2. *The energy E is invariant under the flow of L*

Proof.

$$\begin{aligned}
\frac{dE}{dt}(q(t),\dot{q}(t)) &= \frac{\partial^2 L}{\partial \dot{q}^2}(\ddot{q}(t),\dot{q}(t)) + \frac{\partial^2 L}{\partial q \partial \dot{q}}(\dot{q}(t),\dot{q}(t)) + \frac{\partial L}{\partial \dot{q}}\ddot{q}(t) \\
&\quad - \frac{\partial L}{\partial q}\dot{q}(t) - \frac{\partial L}{\partial \dot{q}}\ddot{q}(t) \\
&= \frac{\partial^2 L}{\partial \dot{q}^2}(\ddot{q}(t),\dot{q}(t)) + \frac{\partial^2 L}{\partial q \partial \dot{q}}(\dot{q}(t),\dot{q}(t)) - \frac{\partial L}{\partial q}\dot{q}(t). \\
\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} &= \frac{\partial^2 L}{\partial \dot{q} \partial \dot{q}}\ddot{q} + \frac{\partial^2 L}{\partial q \partial \dot{q}}\dot{q} - \frac{\partial L}{\partial q} = 0. \\
\implies \frac{dE}{dt}(q(t),\dot{q}(t)) &= 0.
\end{aligned}$$

$\square$

Example 2 (Mass-Spring system continued)**.** For the Mass-Spring system, energy E is given by

$$\begin{aligned} E(q,\dot{q}) &= (2M\dot{q})^T\dot{q} - \dot{q}^T M\dot{q} + q^T K q \\ &= \dot{q}^T M\dot{q} + q^T K q \end{aligned}$$

In this case, the Energy function is indeed the Total Energy of the Mass-Spring system.

$$\begin{aligned} \frac{dE}{dt}(q(t),\dot{q}(t)) &= 2\dot{q}^T(t)M\ddot{q}(t) + 2q^T(t)K\dot{q}(t) \\ &= 2q^T(t)(M\ddot{q}(t) + K\dot{q}(t)) \\ &= 0 \end{aligned}$$

2.2.2 Lagrangian Symplectic form

The Lagrangian Symplectic form $\Omega_L : TQ \mapsto T^*(TQ)$ is given by

$$\Omega_L(q,\dot{q}) = \frac{\partial^2 L}{\partial q^i \partial \dot{q}^j}\mathbf{d}q^i \wedge \mathbf{d}q^j + \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}\mathbf{d}\dot{q}^i \wedge \mathbf{d}q^j \tag{2.5}$$

Theorem 3. *The Lagrangian flow preserves the Lagrangian Symplectic form, i.e.*

$$(F_L^T)^*(\Omega_L) = \Omega_L,\ \forall T \in \mathbb{R}.$$

For a proof of theorem 3, we refer the reader to [MW01, Section 1.2.3].

Example 3 (Mass-Spring system continued)**.** Consider the Lagrangian

$$L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M\dot{q} - \frac{1}{2}q^T K q$$

Then, the Lagrangian Symplectic form is given by

$$\Omega_L(q,\dot{q}) = M_{ij}\mathbf{d}\dot{q}^i \wedge \mathbf{d}q^j$$

Remark 2. The definition of the Lagrangian symplectic form seems rather cryptic and non-intuitive. It is not at all clear what the physical significance of the Lagrangian symplectic form is. However, as we mentioned in Remark

1, there exists a counterpart to the Lagrangian symplectic form on the phase space, which has a very nice geometric interpretation. It can be shown that

$$\Omega_L = (\mathbb{F}L)^* \Omega, \tag{2.6}$$

where Ω is the Liouville form on T^*Q given by

$$\Omega(q, p) = \mathbf{d}q^i \wedge \mathbf{d}p^i.$$

So, the fact that the Lagrangian flow preserves the Lagrangian symplectic form implies that it also preserves Liouville form on the phase space. This means that the Lagrangian flow preserves the area of any 2 dimensional smooth surface in the phase space. For a more detailed discussion on this, and a detailed proof of what we have mentioned above, please see [HLW06, Section VI.2].

With this remark, we end our discussion on continuous time Lagrangian mechanics. There is another important invariant of the Lagrangian flow, the momentum map. In the context of Structural dynamics, except in the case of very simple examples, we usually won't be able to find a momentum map. Because of this, and for the sake of brevity, we shall not be looking at momentum maps and their invariance in this article. We refer the interested reader to [MW01, Section 1.2.4].

Chapter 3

Discrete Lagrangian Mechanics and Variational Integrators

3.1 Basic Definitions

We define a Discrete Lagrangian on a configuration space Q to be a C^2 smooth function $L_d : Q \times Q \mapsto \mathbb{R}$. In practice, L_d is obtained as a discrete approximation of a continuous Lagrangian L. We shall see this in an example. Since we have defined a discretization of the Lagrangian, it is quite natural to now look for a discretization of the action integral. We define the action sum $S_d : Q^{N+1} \mapsto \mathbb{R}$ to be

$$S_d(q) = \sum_{k=0}^{N} L_d(q_k, q_{k+1})$$

We say that the discrete trajectory $\{q_k\}_{k=0}^{N}$ satisfies the *Discrete Euler Lagrange (DEL) equations* if

$$D_1 L_d(q_{k+1}, q_{k+2}) + D_2 L_d(q_k, q_{k+1}) = 0 \tag{3.1}$$

for all $k = 1, ..., N-1$, where $D_i L_d$ is the partial derivative with respect to the i^{th} argument. We define the discrete evolution operator $\phi : Q \times Q \mapsto Q \times Q$ as

$$D_1 L_d(\phi(q_k, q_{k+1})) + D_2 L_d(q_k, q_{k+1}) = 0. \tag{3.2}$$

It is not obvious that given any L_d one can find a discrete evolution operator, because it is not necessary that $D_1 L_d$ is invertible. Under some regularity assumptions on L_d one can indeed show that if q_{k+1} is close enough to q_k then $\phi(q_k, q_{k+1})$ is well defined. For small enough time steps, q_{k+1} will be close enough to q_k and thus the discrete evolution operator will be well defined.

We define the discrete Fiber derivative (or discrete Legendre transform) $\mathbb{F}L_d : Q \times Q \mapsto T^*Q$ given by

$$\mathbb{F}L_d(q_0, q_1) = (q_1, D_2 L_d(q_0, q_1))$$

Example 4. Recall the Lagrangian L defined in Example 1. Consider the Discrete Lagrangian $L_d^\alpha : Q \times Q \mapsto \mathbb{R}$ given by

$$L_d^\alpha(q_0, q_1) = hL\big((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}\big) \tag{3.3}$$

where $h \in \mathbb{R}_+$ is the time step and α is an interpolation parameter. Using the given form of L, we get

$$\begin{aligned}
L_d^\alpha(q_0, q_1) &= h\frac{1}{2}\big(\frac{q_1 - q_0}{h}\big)^T M\big(\frac{q_1 - q_0}{h}\big) - h\frac{1}{2}((1-\alpha)q_0 + \alpha q_1)^T K((1-\alpha)q_0 + \alpha q_1), \\
D_2 L_d^\alpha(q_0, q_1) &= \frac{1}{h}M(q_1 - q_0) - h\alpha K((1-\alpha)q_0 + \alpha q_1), \\
D_1 L_d^\alpha(q_1, q_2) &= \frac{1}{h}M(q_1 - q_2) - h(1-\alpha)K((1-\alpha)q_1 + \alpha q_2).
\end{aligned}$$

$$\begin{aligned}
&D_2 L_d^\alpha(q_0, q_1) + D_1 L_d^\alpha(q_1, q_2) = 0 \\
&\iff -(M + h^2\alpha(1-\alpha)K)q_2 + M(2q_1 - q_0) - h^2 K\big(\alpha(1-\alpha)q_0 + (\alpha^2 + (1-\alpha)^2)q_1\big) = 0 \\
&\iff (M + h^2\alpha(1-\alpha)K)q_2 = M(2q_1 - q_0) - h^2 K\big(\alpha(1-\alpha)q_0 + (\alpha^2 + (1-\alpha)^2)q_1\big) \\
&\iff q_2 = (M + h^2\alpha(1-\alpha)K)^{-1}\big(M(2q_1 - q_0) - h^2 K\big(\alpha(1-\alpha)q_0 + (\alpha^2 + (1-\alpha)^2)q_1\big)\big).
\end{aligned}$$

$$\therefore \phi(q_0, q_1) = (q_1, (M + h^2\alpha(1-\alpha)K)^{-1}\big(M(2q_1 - q_0) - h^2 K\big(\alpha(1-\alpha)q_0 + (\alpha^2 + (1-\alpha)^2)q_1\big)\big))$$

The discrete Fiber derivative is given by

$$\mathbb{F}L_d^\alpha(q_0, q_1) = (q_1, M\big(\frac{q_1 - q_0}{h}\big) - h\alpha K((1-\alpha)q_0 + \alpha q_1))$$

3.2 Invariants of the discrete flow

3.2.1 Discrete Lagrangian Energy

The energy associated with a discrete Lagrangian is given by

$$E_d(q_0, q_1, h) = -\frac{\partial}{\partial h}L_d(q_0, q_1, h) \tag{3.4}$$

Even though we defined the discrete Lagrangian to be a function of just two arguments, it did contain the time-step as a third argument. The author apologizes for this abuse of notation.

Example 5. For the discrete Lagrangian given in Example 4, the energy is given by

$$E_d^\alpha(q_0, q_1) = \frac{1}{2}\big(\frac{q_1 - q_0}{h}\big)^T M\big(\frac{q_1 - q_0}{h}\big) + \frac{1}{2}((1-\alpha)q_0 + \alpha q_1)^T K((1-\alpha)q_0 + \alpha q_1).$$

In fact, in this example, we can write

$$E_d^\alpha(q_0, q_1) = E((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}).$$

where E is the energy associated with the Lagrangian L.

3.2.2 Discrete Lagrangian Symplectic form

The Discrete Lagrangian Symplectic form $\Omega_{L_d} : Q \times Q \mapsto T^*(Q \times Q)$ is given by

$$\Omega_{L_d}(q_0, q_1) = \frac{\partial^2 L_d}{\partial q_0^i \partial q_0^j}(q_0, q_1)\mathbf{d}q_0^i \wedge \mathbf{d}q_1^j \tag{3.5}$$

Theorem 4. *The Discrete Lagrangian evolution operator ϕ preserves the Discrete Lagrangian symplectic form, i.e.*

$$\phi^* \Omega_{L_d} = \Omega_{L_d} \tag{3.6}$$

For a proof of theorem 4 we refer the reader to [MW01, Section 1.3.2].

Example 6. For the discrete Lagrangian given in Example 4, the discrete Lagrangian symplectic form is given by

$$\Omega_{L_d^\alpha}(q_0, q_1) = -(\frac{1}{h}M_{ij} + h\alpha(1-\alpha)K_{ij})\mathbf{d}q_0^i \wedge \mathbf{d}q_1^j \tag{3.7}$$

Remark 3. Just like in the continuous case, we can show here also that

$$\Omega_{L_d} = (\mathbb{F}L_d)^* \Omega, \tag{3.8}$$

where Ω is the Liouville form on T^*Q (See [MW01, Section 1.5.1] for a proof). So, in discrete time also we have a similar interpretation of the invariance of the symplectic form under the flow as in Remark 2.

3.3 Variational Integrators

Suppose we have a mechanical system evolving on Q with Lagrangian L. The reader might already have guessed how we go about constructing Variational integrators. What we would like is the discrete action sum to approximate the action integral, which can be restated as

$$L_d(q_0, q_1, h) \approx \int_0^h L(q_{EL}(t), \dot{q}_{EL}(t)) \tag{3.9}$$

where $q_{EL}(t)$ is the curve satisfying the EL equations and $q_{EL}(0) = q_0, q_{EL}(h) = q_1$. The solution to the DEL equations corresponding to L_d is what we expect will give us an approximation of the continuous EL trajectory.

In the preceding sections, the reader might have noticed that our presentation has almost mirrored that in the continuous time case. The only thing which did not have a discrete time correspondence is the Hamilton's principle. We shall fill this void here. We first define the Exact Discrete Lagrangian $L_d^E : TQ \mapsto \mathbb{R}$ as

$$L_d^E(q_0, q_1, h) = \int_0^h L(q_{EL}(t), \dot{q}_{EL}(t)) \tag{3.10}$$

where $q_{EL}(t)$ is the curve satisfying the EL equations and $q_{EL}(0) = q_0, q_{EL}(h) = q_1$. The solution to the DEL equations corresponding to L_d is what we expect will give us an approximation of the continuous EL trajectory.

Theorem 5. *A discrete trajectory $\{q_k\}_{k=0}^N$ satisfies the DEL equations corresponding to L_d^E iff there exists a continuous trajectory $q(t)$ satisfying the EL equations corresponding to L such $q_k = q(kh)$.*

For a proof of Theorem 5, we refer the reader to [MW01, Section 1.6]. What we would like to highlight here is that if know L_d^E, then by solving the DEL equations we can find an *exact* discretization of the original continuous time trajectory. It might seem like we have found the most ideal integrator ever; unfortunately this is not the case. It is virtually impossible to find L_d^E for any non-trivial problem. Nevertheless, the exact discrete Lagrangian is an important object in the error analysis of variational integrators.). Many important properties of the integrator, like convergence and order, can be expresses in terms of the error between the chosen discrete Lagrangian L_d and the exact discrete Lagrangian L_d^E (See [MW01, Chapter 2].

We have already seen a class of Variational integrators for the Mass-Spring system in Example 4. We will end this chapter with the construction of another class of variational integrators. It is to be noted that the expression for the discrete evolution operator in Example 4 is rather long and unwieldy. To avoid this, we introduce the evaluated acceleration notation :

$$a_{k+\alpha} = -M^{-1}(K((1-\alpha)q_k + \alpha q_{k+1})) \tag{3.11}$$

With this, we can rewrite the expression in Example 4 as

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = (1-\alpha)a_{k+1+\alpha} + \alpha a_{k+\alpha} \tag{3.12}$$

Now we define the new family of integrators

$$L_d^{sym,\alpha}(q_0, q_1) = \frac{h}{2}L((1-\alpha)q_0 + \alpha q_1, \frac{q_1 - q_0}{h}) + \frac{h}{2}L(\alpha q_0 + (1-\alpha)q_1, \frac{q_1 - q_0}{h}) \tag{3.13}$$

It can be easily seen that the DEL equations corresponding to $L_d^{sym,\alpha}$ is

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = \frac{1}{2}((1-\alpha)a_{k+1+\alpha} + \alpha a_{k+2-\alpha} + \alpha a_{k+\alpha} + (1-\alpha)a_{k+1-\alpha}) \tag{3.14}$$

Chapter 4

The Newmark Algorithm

We finally get to the crux of this article, the Newmark method. In this section we will introduce the Newmark family of time integration algorithms for mechanical systems with Lagrangian L of the form

$$L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M\dot{q} - \frac{1}{2}q^T Kq,\ M = M^T \succ 0, K = K^T \succeq 0. \tag{4.1}$$

We will then go on to prove that the Newmark family of integrators are variational in nature. We will then discuss some implications of this. In the next chapter, we will verify through simulations the properties we prove in this section.

4.1 Newmark Schemes

We have already shown that the EL equations corresponding to the Lagrangian 4.1 is given by

$$M\ddot{q} + Kq = 0 \tag{4.2}$$

The Newmark method with constants $0 \leq \gamma \leq 1, 0 \leq \beta \leq \frac{1}{2}$ is given by

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}((1-2\beta)a_k + 2\beta a_{k+1}) \tag{4.3}$$

$$\dot{q}_{k+1} = \dot{q}_k + h((1-\gamma)a_k + \gamma a_{k+1}) \tag{4.4}$$

$$\tag{4.5}$$

where

$$a_k = -M^{-1}Kq_k \tag{4.6}$$

In equation 4.3, we have written the algorithm as an update of position of velocity. We shall rewrite the algorithm as an update of position alone.

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}((1-2\beta)a_k + 2\beta a_{k+1}) \tag{4.7}$$

$$q_{k+2} = q_{k+1} + h\dot{q}_{k+1} + \frac{h^2}{2}((1-2\beta)a_{k+1} + 2\beta a_{k+2}) \tag{4.8}$$

$$\implies q_{k+2} - q_{k+1} = q_{k+1} - q_k + h(\dot{q}_{k+1} - \dot{q}_k) \tag{4.9}$$

$$+ \frac{h^2}{2}((1-2\beta)(a_{k+1} - a_k) + 2\beta(a_{k+2} - a_{k+1}))$$

$$= q_{k+1} - q_k + h^2((1-\gamma)a_k + \gamma a_{k+1}) \tag{4.10}$$

$$+ \frac{h^2}{2}((1-2\beta)(a_{k+1} - a_k) + 2\beta(a_{k+2} - a_{k+1})) \tag{4.11}$$

Therefore, the Newmark algorithm in the configuration update form is

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = (\frac{1}{2} - \gamma + \beta)a_k + (\frac{1}{2} + \gamma - 2\beta)a_{k+1} + \beta a_{k+2} \tag{4.12}$$

It is well known that for the Newmark method is second-order accurate if and only if $\gamma = \frac{1}{2}$, otherwise it is only consistent. Thus, γ is usually taken equal to $\frac{1}{2}$. We will prove the equivalence of Newmark methods with $\gamma = \frac{1}{2}$ and variational methods in two stages :

1. We first show that for $\gamma = \frac{1}{2}$ and any $\beta \leq \frac{1}{4}$, the Newmark method is equivalent to the variational method with discrete Lagrangian $L_d^{sym,\alpha}$ where α is chosen so that $\beta = \alpha(1-\alpha)$. This is relatively easy to show, as it follows from simple comparison between equations 4.12 and 3.14.

2. We will then establish that for $\gamma = \frac{1}{2}$ and any $0 \leq \beta \leq \frac{1}{2}$, there exists a discrete Lagrangian $L_d^{nm,\beta}$ such that the variational integrator corresponding to $L_d^{nm,\beta}$ is the same as the Newmark method.

4.1.1 Newmark with $\gamma = \frac{1}{2}$ and $0 \leq \beta \leq \frac{1}{4}$

Theorem 6. *Newmark method with $\gamma = \frac{1}{2}$ and $\beta \leq \frac{1}{4}$ is equivalent to the $L_d^{sym,\alpha}$ variational algorithm with α chosen such that $\beta = \alpha(1-\alpha)$.*

Proof. We recall the $L_d^{sym,\alpha}$ update 3.14

$$\begin{aligned}\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) &= \frac{1}{2}((1-\alpha)a_{k+1+\alpha} + \alpha a_{k+2-\alpha} + \alpha a_{k+\alpha} + (1-\alpha)a_{k+1-\alpha}) \\ &= \alpha(1-\alpha)a_k + (\alpha^2 + (1-\alpha)^2)a_{k+1} + \alpha(1-\alpha)a_{k+2}\end{aligned} \tag{4.13}$$

When $\gamma = \frac{1}{2}$ the Newmark update can be written as

$$\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = \beta a_k + (1-2\beta)a_{k+1} + \beta a_{k+2} \tag{4.14}$$

Comparing 4.13 and 4.14, we see that if $\beta = \alpha(1-\alpha)$, the Newmark method and $L_d^{sym,\alpha}$ method are the same. Since $\beta \leq \frac{1}{4}$, we can find an $\alpha \in [0,1]$ such that $\beta = \alpha(1-\alpha)$. □

We recall some popular methods which belong to this class.

1. $\gamma = \frac{1}{2}, \beta = 0$: The Newmark algorithm in velocity update form can be written as

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2}a_k \tag{4.15}$$

$$\dot{q}_{k+1} = \dot{q}_k + \frac{h}{2}(a_k + a_{k+1}) \tag{4.16}$$

(4.17)

   This is the well known *Central difference scheme*.
   When $\beta = 0, \alpha(1-\alpha) = \beta \implies \alpha = 0$. So, the central difference scheme is equivalent to the the variational $L_d^{sym,\alpha}(\alpha = 0)$ algorithm.

2. $\gamma = \frac{1}{2}, \beta = \frac{1}{4}$: The Newmark algorithm in velocity update form can be written as

$$q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{4}(a_k + a_{k+1}) \tag{4.18}$$

$$\dot{q}_{k+1} = \dot{q}_k + \frac{h}{2}(a_k + a_{k+1}) \tag{4.19}$$

(4.20)

   This is the well known *Average acceleration method*.
   When $\beta = \frac{1}{4}, \alpha(1-\alpha) = \beta \implies \alpha = \frac{1}{2}$. So, the average acceleration method is equivalent to the the variational $L_d^{sym,\alpha}(\alpha = \frac{1}{2})$ algorithm.

4.1.2 Newmark with $\gamma = \frac{1}{2}$ and $0 \leq \beta \leq \frac{1}{2}$

In this section, we will prove that the Newmark method is variational in the more general case, where $0 \leq \beta \leq \frac{1}{2}$. To this end, consider the coordinate transformation

$$x_k = q_k + \beta h^2 M^{-1} K q_k \tag{4.21}$$
$$= (I + \beta h^2 M^{-1} K) q_k \tag{4.22}$$
$$= A^{h,\beta} q_k. \tag{4.23}$$

where $A^{h,\beta} = I + \beta h^2 M^{-1} K$. For small enough h, $A^{h,\beta}$ is an invertible transformation.

Theorem 7. *Consider the discrete Lagrangian $L_d^{nm,\beta}$ given by*

$$L_d^{nm,\beta}(q_0, q_1) = \frac{h}{2}\Big(\frac{q_1 - q_0}{h}\Big)^T \big(A^{h,\beta}\big)^T M \big(A^{h,\beta}\big)\Big(\frac{q_1 - q_0}{h}\Big) - h q_0^T \big(A^{h,\beta}\big)^T K q_0. \tag{4.24}$$

Then the $L_d^{nm,\beta}$ variational algorithm is equivalent to the Newmark algorithm with $\gamma = \frac{1}{2}$ and $0 \leq \beta \leq \frac{1}{2}$.

Proof. We first rewrite the Newmark update scheme given in Equation 4.12 in terms of x_k. When $\gamma = \frac{1}{2}$, 4.12 can be written as

$$\begin{aligned}
&\frac{1}{h^2}(q_{k+2} - 2q_{k+1} + q_k) = \beta a_k + (1 - 2\beta) a_{k+1} + \beta a_{k+2} \\
\Longrightarrow\ & (q_{k+2} - \beta h^2 a_{k+2}) - 2(q_{k+1} - \beta h^2 a_{k+1}) + (q_k - \beta h^2 a_k) = h^2 a_{k+1} \\
\Longrightarrow\ & (I + \beta h^2 M^{-1} K) q_{k+2} - 2(I + \beta h^2 M^{-1} K) q_{k+1} \\
& + (I + \beta h^2 M^{-1} K) q_k = -h^2 M^{-1} K q_{k+1} \\
\Longrightarrow\ & A^{h,\beta} q_{k+2} - 2A^{h,\beta} q_{k+1} + A^{h,\beta} q_k + h^2 M^{-1} K q_{k+1} = 0.
\end{aligned}$$

Now, if we look at the DEL equations corresponding to $L_d^{nm,\beta}$, we get

$$\begin{aligned}
&\big(A^{h,\beta}\big)^T M \big(A^{h,\beta}\big)(2q_{k+1} - q_k - q_{k+2}) - h^2 \big(A^{h,\beta}\big)^T K q_{k+1} = 0 \\
\Longrightarrow\ & M\big(A^{h,\beta}\big)(2q_{k+1} - q_k - q_{k+2}) - h^2 K q_{k+1} = 0 \\
\Longrightarrow\ & \big(A^{h,\beta}\big)(2q_{k+1} - q_k - q_{k+2}) - h^2 M^{-1} K q_{k+1} \\
\Longrightarrow\ & \big(A^{h,\beta}\big)(q_{k+2} - 2q_{k+1} + q_k) + h^2 M^{-1} K q_{k+1} = 0
\end{aligned}$$

Therefore, we see that the DEL equations and the Newmark update equations are the same. □

In conclusion, we have shown that all members of the Newmark family with $\gamma = \frac{1}{2}$ are equivalent to a Variational integrator. This means that the Newmark algorithms are symplectic, and preserve the corresponding symplectic form on the phase space and the discrete Lagrangian energy. We shall see this in action in the next chapter, where we present the simulation results on a 100,000 DOF mechanical system.

Chapter 5

Results and Discussions

We finally verify all the theory that we've developed in the preceding chapters. We observe the energy behaviour of various time integration algorithms applied to a conservative mechanical system. As expected, the variational algorithms display excellent energy behaviour, even for long integration periods.

5.1 Simulation results

The system we consider here is a linear mass-spring chain with 100,000 mass elements. It is initialized with a random configuration and velocity value in each DOF between 2 and 5. The algorithms whose energy behaviour we compare here are:

- Linear acceleration method (Newmark method with $\beta = 0.25, \gamma = 0.5$).
- Central difference method (Newmark method with $\beta = 0, \gamma = 0.5$).
- Newmark method with $\beta = 0.6, \gamma = 0.5$.
- Fourth order Runge Kutta with fixed time-step.

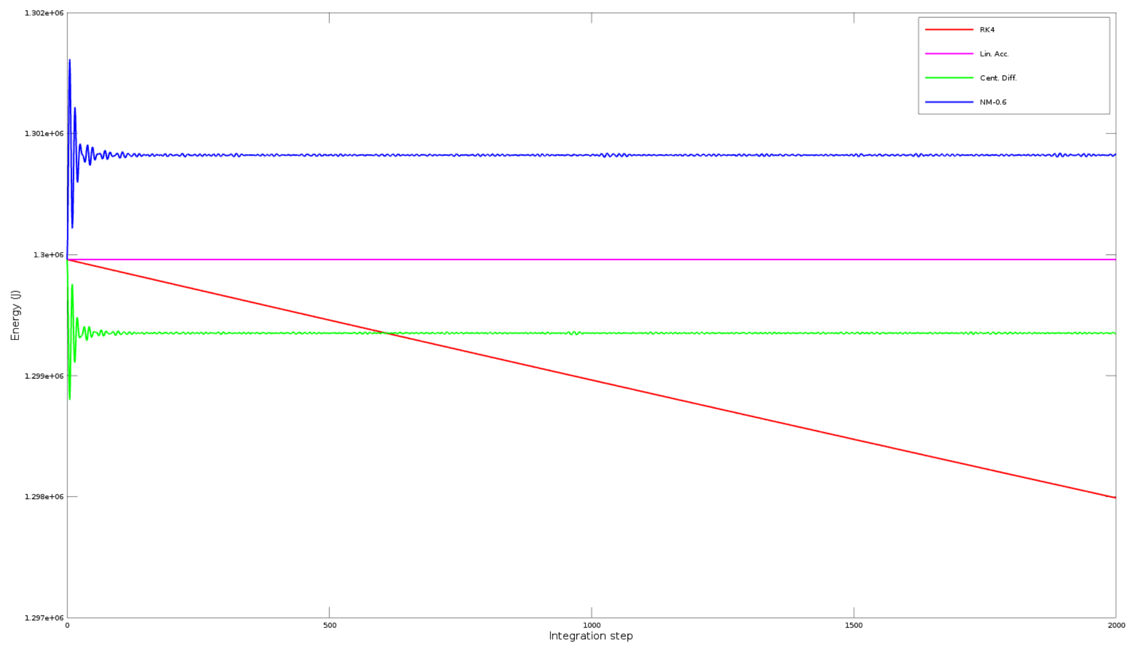

Figure 5.1: Energy behaviour of different time integration algorithms

The simulation results are shown in figure 5.1. We have plotted the total energy of the system with time for the 4 integration algorithms mentioned above. The pink, green, blue and red line shows the energy of the trajectories generated by Linear acceleration, Central difference, Newmark with $\beta = 0.6$ and RK-4 method respectively.

5.2 Discussions

As expected, due to the variational derivation of the first three algorithms, they display excellent global energy behaviour, while RK 4 method induces artificial damping to the system. The exceptional behaviour of the Linear acceleration method deserves special mention; it almost **exactly** preserves energy (very small oscillations were observed upon zooming). Central difference and the Newmark method with $\beta = 0.6$ oscillates a bit in the beginning but quickly settles to a value not far away from the initial energy. This is because the algorithm preserves not the true energy of the system, but the discrete Lagrangian energy given in 3.4. But the Runge Kutta method of order 4 introduces an artificial linear damping of energy; the energy decreases linearly with time. In fact, the RK-4 method introduces this linear damping regardless of how small a step-size one chooses, though the rate of damping does decrease with decreasing step-size. For integrating conservative systems over long periods of time, this might be a problem. It is to be noted that the RK method is of order 4 while the other methods are order 2. Despite this, the variational nature of derivation endows them with much better energy behaviour.

Throughout the article, we were only interested in the extent to which integrators preserved invariants of the system. However, ultimately, what would matter the most to one is the accuracy of the trajectory generated by the integrator. These are two related issues, but not entirely the same. It is true that in a lot of case, symplectic integrators exhibit improved trajectory accuracy, but we give no such guarantee in this article. However, the author expects symplectic methods to perform well in the case of conservative systems because they take good care of the main conservative part of these systems, and this is where most traditional algorithms introduce most of the error.

Chapter 6

Conclusions

In conclusion, we summarize the main achievements of this article.

- We defined what it means for an integration scheme to be variational.
- We showed how such variational schemes preserve certain invariants of the system.
- We proved that the Newmark family of methods with $\gamma = \frac{1}{2}$ are variational in nature.
- We validated through numerical simulations that the Newmark methods exactly preserve the energy of a conservative mechanical system, even better than higher order schemes.
- We explained why this is the reason that symplectic integrators exhibit improved trajectory accuracy in the case of conservative mechanical systems.

Although the work presented in this article is mainly based on [KMOW00], we have only shown a fraction of the work done there. They have shown that the Newmark methods are variational for a more general class of mechanical systems with nonlinear potentials, we have only considered the case where the potential is quadratic. They also go on to extend the theory of variational integrators to systems with dissipation and forcing. They also discuss another important invariant of Lagrangian systems: the momentum map. For the sake of brevity, and relevance to structural dynamics, the author has chosen to avoid presenting all these topics in this article. However, it is the author's belief that this article has been successful in presenting the essential ideas behind variational integrators and their link to the Newmark family of methods used in structural dynamics.

The author would like to end with a disclaimer : **The author claims no credit for the development of the theory presented in the article.** As mentioned before, most of it can be found in [KMOW00] and [MW01]. The simulations were performed by the author itself. Apart from this, the author has made efforts to include whatever little insight the author has in the area to provide more intuitive explanations wherever possible and make the article a little more accessible to the reader.

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