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# A space-time geodesic approach for phase fitted variational integrators

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**Abstract.** The use of space-time geodesic approach of classical mechanics is investigated, in order to derive time adaptive high order phase fitted variational integrators. The proposed technique is employed for systems of which the Lagrangian is of separable form. To this end, first the unfolding of the standard Euler-Lagrange system to its space-time manifold is presented and then it is rewritten as a geodesic problem with zero potential energy. Preliminary simulation results (without optimizing the choice of step sizing) show that one can use the space-time geodesic formulation to generate an adaptive scheme that still preserves some underlying geometric structure.

## 1. Introduction

In recent years, in order to reduce computational cost, time adaptivity is an important ingredient. Therefore adaptive time integration schemes for ordinary differential equations (ODEs) have been well established. Although they perform extremely well for many applications, for problems involving the integration of Hamiltonian systems, there are good reasons for using symplectic integrators [1, 2].

On that end, studies have been done in order to derive and analyze symplectic integrators with variable time steps, but the early results were not promising [3, 4, 5]. Among these, there have been two types of time variation steps. In the first set of studies, the time step varies explicitly as the time is running resulting to problems. In the second set of studies, the time step was chosen using the dynamical variables of the system  $q, p$ , i.e.  $\Delta t = \Delta(q, p)$ . Using this choice of  $\Delta t$ , the equations are no longer in canonical Hamiltonian form (but rather Hamiltonian in non-canonical variables) and quite unreliable results are obtained. The results in both cases lead to the conclusion that if one needs an adaptive time step integrator is forced to use a high order non-symplectic scheme [6, 7].

In this paper, the Galerkin type, high order symplectic integrators of [8, 9, 10, 11, 12, 13, 14] are extended through the use of adaptive time stepping. To this end, in addition to the spacetime view point of [1, 2], the geodesic viewpoint [15, 16] is regarded in order to understand and overcome the problems appeared in the application of symplectic integrators with variable time steps. One of our purposes is to derive a method of optimal time-step adaptation scheme.

## 2. Geodesic approach

In order to construct time adaptive integrators, the Lagrangian function  $L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - V(x)$  ( $x \in \mathbb{R}$ ) must be considered. For the latter Lagrangian, the corresponding Euler-Lagrange



equation is

$$\ddot{x} = -\frac{\partial V}{\partial x}. \tag{1}$$

Choosing initial conditions  $x_0 = x(0)$  and  $\dot{x}_0 = \dot{x}(0)$ ,  $x(t)$  can be considered as a solution of (1) for some time interval  $t \in [0, T]$ .

We they consider the Lagrangian  $\tilde{L} = \frac{1}{2}\dot{x}^2 + \frac{1}{2V}t^2$ , where the primes in  $\dot{x}$  denote differentiation with respect to some parameter  $\lambda$ , see [15]. The corresponding Euler-Lagrange equations and initial conditions are

$$x'' = -\frac{1}{2V^2} \frac{\partial V}{\partial x} t'^2, \quad x_0 = x(0), \quad x'_0 = \dot{x}_0 t'_0 \tag{2a}$$

$$t'' = \frac{1}{V} \frac{\partial V}{\partial x} t' x', \quad t_0 = 0, \quad t'(0) = \alpha V(x_0). \tag{2b}$$

Even though  $\tilde{L}$  depends upon  $V$  and couples the space and time variables in a non trivial manner, the embedded evolution equations for  $x$  only depend on  $\partial V/\partial x$ . Of course one could add any constant to  $V$  without changing the  $x$ -dynamics [16].

It can be proved, see e.g. [15, 16], that if  $\tilde{x}(\lambda), t(\lambda)$  solve (2b) because, some time interval  $\lambda \in [0, \tilde{T}]$ , then  $\tilde{x}(\lambda) = x(2t/\sqrt{\alpha})$  for as long as both sides are defined i.e. the solutions for  $x$  and  $\tilde{x}$  differ only by a constant that rescales the time. The discrete version of the above statement also holds true [16].

We now consider the following two Lagrangians [15, 16]

$$L_1 = \sqrt{\dot{x}^2 + f(x)t^2}, \quad L_2 = \frac{1}{2} (\dot{x}^2 + f(x)t^2). \tag{3}$$

The action corresponding to  $L_1$  is invariant under arbitrary reparametrization of  $\lambda$ , whereas the  $L_2$  action is only affine reparametrization invariant, therefore, the Euler-Lagrange equations corresponding to  $L_2$  are affine time reparametrization invariant [16]. The Euler-Lagrange equations corresponding to  $L_1$  are

$$\frac{d}{d\lambda} \left( \frac{\dot{x}}{\sqrt{\dot{x}^2 + f(x)t^2}} \right) = -\frac{t^2}{2\sqrt{\dot{x}^2 + f(x)t^2}} \frac{\partial f}{\partial x} \tag{4a}$$

$$\frac{d}{d\lambda} \left( \frac{f(x)\dot{x}}{\sqrt{\dot{x}^2 + f(x)t^2}} \right) = 0. \tag{4b}$$

Equations (4) are reparametrization invariant, see [16]. Notice also that the equations in (4) look like two evolution equations which should, in general, provide us not only the shape of the curve but also the parametrization of the curve.

### 3. Review of phase fitted variational integrators

As it is known, for the derivation of high order variational integrators, we need to apply discrete variational calculus [8, 9, 10]. As usually, a discrete Lagrangian, is a map  $L_d : Q \times Q \rightarrow \mathbb{R}$  which may be considered as an approximation of a continuous action obtained through the Lagrangian  $L : TQ \rightarrow \mathbb{R}$ , i.e.

$$L_d(q_k, q_{k+1}, h_k) \approx \int_{t_k}^{t_{k+1}} L(q, \dot{q}) dt. \tag{5}$$

The action sum  $S_d : Q^{N+1} \rightarrow \mathbb{R}$ ,  $N \in \mathbb{N}$  corresponding to the Lagrangian  $L_d$  is defined as

$$S_d(\gamma_d) = \sum_{k=0}^{N-1} h_k L_d(q_k, q_{k+1}, h_k), \quad (6)$$

with  $\gamma_d = (q_0, \dots, q_N)$  denoting the discrete trajectory. For any covector  $\alpha \in T_{(x_1, x_2)}^*(Q \times Q)$  we have the decomposition  $\alpha = \alpha_1 + \alpha_2$ , where  $\alpha_i \in T_{x_i}^*(Q \times Q)$ . Thus,  $dL_d(q_0, q_1) = D_1 L_d(q_0, q_1) + D_2 L_d(q_0, q_1)$ , where the notation  $D_i L_d$  indicates the slot derivative with respect to the  $i$ -argument of  $L_d$ . According to the discrete variational principle, as usually the solutions of the discrete system are determined from  $L_d$  by extremizing the action sum for given fixed points  $q_0$  and  $q_N$ . Extremizing  $S_d$  over all the intermediate points of  $\gamma_d$ , the system of difference equations

$$h_{k-1} D_2 L_d(q_{k-1}, q_k, h_{k-1}) + h_k D_1 L_d(q_k, q_{k+1}, h_k) = 0, \quad k = 1, \dots, N-1, \quad (7)$$

are obtained which are commonly called the discrete Euler-Lagrange equations.

To derive high order methods, we approximate the action integral along the curve segment between  $q_k$  and  $q_{k+1}$  using a discrete Lagrangian that depends only on the end points. This way we obtain expressions for the configurations  $q_k^j$  and velocities  $\dot{q}_k^j$ ,  $j = 0, \dots, S-1$ ,  $S \in \mathbb{N}$ , at time  $t_k^j \in [t_k, t_{k+1}]$ . Then, by expressing  $t_k^j$  as  $t_k^j = t_k + C_k^j h_k$  for  $C_k^j \in [0, 1]$  such that  $C_k^0 = 0$ ,  $C_k^{S-1} = 1$  we write

$$q_k^j = g_1(t_k^j) q_k + g_2(t_k^j) q_{k+1}, \quad \dot{q}_k^j = \dot{g}_1(t_k^j) q_k + \dot{g}_2(t_k^j) q_{k+1}, \quad (8)$$

where  $h \in \mathbb{R}$  is the time step. We next choose the functions

$$g_1(t_k^j) = \sin\left(u - \frac{t_k^j - t_k}{h_k} u\right) (\sin u)^{-1}, \quad g_2(t_k^j) = \sin\left(\frac{t_k^j - t_k}{h_k} u\right) (\sin u)^{-1}, \quad (9)$$

to represent the oscillatory behavior of the solution [11, 12, 13, 14, 17]. For the sake of continuity the conditions  $g_1(t_{k+1}) = g_2(t_k) = 0$  and  $g_1(t_k) = g_2(t_{k+1}) = 1$  are required.

For any different choice of interpolation assumed we define the discrete Lagrangian by the weighted sum (see [11])

$$L_d(q_k, q_{k+1}, h_k) = \sum_{j=0}^{S-1} h_k w^j L(q(t_k^j), \dot{q}(t_k^j)), \quad (10)$$

where, as can be easily proved,  $\sum_{j=0}^{S-1} w^j (C_k^j)^m = \frac{1}{m+1}$ , with  $m = 0, 1, \dots, S-1$  and  $k = 0, 1, \dots, N-1$  [11, 12].

Applying the above interpolation technique with the trigonometric expressions of (9) and following the phase lag analysis of [11, 12], the parameter  $u$  must be chosen as  $u = \omega h$ . For problems including a definite frequency  $\omega$  (such as the harmonic oscillator) the parameter  $u$  can be easily computed. For the solution of orbital problems of the general  $N$ -body problem, where no unique frequency is given, a new parameter  $u$  must be defined by estimating the frequency of the motion for any moving point mass [12, 13, 14].

#### 4. Time adaptive phase fitted variational integrators

Using (10), for the length action given by  $L_1$  in (3), the corresponding discrete Lagrangian reads

$$L_{1d}(q_k, q_{k+1}, h_k) = \sum_{j=0}^{S-1} h_k w^j \sqrt{\left(\dot{x}_k^j\right)^2 + f\left(x_k^j\right) \left(\dot{t}_k^j\right)^2}, \quad (11)$$

where  $x_k^j$  are defined using (8) and  $\dot{x}_k^j, \dot{t}_k^j$  using the expression

$$\dot{q}_k^j = \frac{\partial q_k^j}{\partial \lambda} = \frac{\partial t}{\partial \lambda} \left( \dot{g}_1(t_k^j) q_k + \dot{g}_2(t_k^j) q_{k+1} \right) = \dot{g}_1(t_k^j) q_k + \dot{g}_2(t_k^j) q_{k+1}. \quad (12)$$

For the latter Lagrangian, the discrete Euler-Lagrange equations (7) give the discrete analogues of (4a) as

$$\begin{aligned} & \sum_{j=0}^{S-1} w^j \frac{h_k}{2d_{k,k-1}} \left[ 2\dot{g}_2(t_k^j) \left( \dot{g}_1(t_k^j) x_{k-1} + \dot{g}_2(t_k^j) x_k \right) + \frac{\partial}{\partial x_k} f \left( g_1(t_k^j) x_{k-1} + g_2(t_k^j) x_k \right) \left( \dot{g}_1(t_k^j) t_{k-1} + \dot{g}_2(t_k^j) t_k \right)^2 \right] \\ & + \sum_{j=0}^{S-1} w^j \frac{h_{k+1}}{2d_{k+1,k}} \left[ 2\dot{g}_1(t_k^j) \left( \dot{g}_1(t_k^j) x_k + \dot{g}_2(t_k^j) x_{k+1} \right) + \frac{\partial}{\partial x_k} f \left( g_1(t_k^j) x_k + g_2(t_k^j) x_{k+1} \right) \left( \dot{g}_1(t_k^j) t_k + \dot{g}_2(t_k^j) t_{k+1} \right)^2 \right] \end{aligned} \quad (13)$$

and of (4b) as

$$\begin{aligned} & \sum_{j=0}^{S-1} w^j \frac{h_k}{d_{k,k-1}} \left[ \dot{g}_2(t_k^j) f \left( g_1(t_k^j) x_{k-1} + g_2(t_k^j) x_k \right) \left( \dot{g}_1(t_k^j) t_{k-1} + \dot{g}_2(t_k^j) t_k \right)^2 \right] \\ & + \sum_{j=0}^{S-1} w^j \frac{h_{k+1}}{d_{k+1,k}} \left[ \dot{g}_1(t_k^j) f \left( g_1(t_k^j) x_k + g_2(t_k^j) x_{k+1} \right) \left( \dot{g}_1(t_k^j) t_k + \dot{g}_2(t_k^j) t_{k+1} \right)^2 \right]. \end{aligned} \quad (14)$$

In these equations  $d_{k+1,k}$  is given by

$$d_{k+1,k} = \sqrt{\left[ \dot{g}_1(t_k^j) x_k + \dot{g}_2(t_k^j) x_{k+1} \right]^2 + f \left( g_1(t_k^j) x_{k-1} + g_2(t_k^j) x_k \right) \left[ \dot{g}_1(t_k^j) t_{k-1} + \dot{g}_2(t_k^j) t_k \right]^2}. \quad (15)$$

and similarly for  $d_{k,k-1}$ .

In accordance with the continuous case, the equations (13) and (14) are not independent. To solve the system above, we can choose arbitrary step sizes in either  $t$  or  $x$  direction and solve for the  $x$  or  $t$ , respectively.

Once we have solved the discrete Euler-Lagrange equations (13) and (14), we get a sequence of points  $(x_0, t_0), \dots, (x_N, t_N)$ , where  $t_0, \dots, t_N$  does not necessarily present the physical time. Using this sequence of points, for the discrete Hamiltonian

$$H_d(x_0, x_1, h_0) = -h_0 D_3 L_d(x_0, x_1, h_0) - L_d(q_0, q_1, h_0) \quad (16)$$

and recalling that the energy expressed by the Hamiltonian is conjugate variable of the physical time, i.e.

$$H_d(x_0, x_1, h_0) = H_d(x_1, x_2, h_1), \quad (17)$$

we reconstruct the physical time.

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