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Local path fitting: A new approach to variational integrators

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ABSTRACT

A new approach for constructing variational integrators is presented. In the general case, the estimation of the action integral in a time interval $[t_k, t_{k+1}]$ is used to construct a symplectic map $(q_k, q_{k+1}) \to (q_{k+1}, q_{k+2})$. The basic idea, is that only the partial derivatives of the estimated action integral of the Lagrangian are needed in the general theory. The analytic calculation of these derivatives, gives rise to a new integral that depends on the Euler–Lagrange vector itself (which in the continuous and exact case vanishes) and not on the Lagrangian. Since this new integral can only be computed through a numerical method based on some internal grid points, we can locally fit the exact curve by demanding the Euler–Lagrange vector to vanish at these grid points. Thus, the integral vanishes, and the process dramatically simplifies the calculation of high order approximations. The new technique is tested in high order solutions of the two-body problem with high eccentricity (up to 0.99) and of the outer planets of the solar system.

1. Introduction

It is well known that the dynamics of conservative systems in mechanics, physics, biology, and chemistry may accurately be described within the Hamiltonian formalism [1,2]. An important property of the Hamiltonian flow (or solution to a Hamiltonian system) is that it preserves the Hamiltonian and the symplectic form (see, for example, Ref. [3]). A key consequence of symplecticity is that the Hamiltonian flow is phase-space volume preserving (Liouville's theorem). Since analytic expressions for the Hamiltonian flow are rarely available, approximations based on time discretization are used [4–6]. A numerical integration method that approximates a Hamiltonian flow is symplectic if it discretely preserves a symplectic 2-form to within numerical round off [2,4,7], otherwise is called standard.

By ignoring the Hamiltonian structure, a standard method often introduces spurious dynamics, an effect which is excellently illustrated in Ref. [8] where the computation of a Poincaré section shows that the standard method artificially corrupts phase space structures by exhibiting a systematic drift in the invariant tori of the spherical pendulum, whereas variational Euler procedure preserves them [9]. Moreover, in systems that are non-integrable, symplectic integrators often operate much better even compared with projection methods, where the calculated values are projected in the manifold defined by the constant symplectic structure. Finally, as shown in Ref. [10], in many body problems, the symplectic integrators perform increasingly better than standard methods as the number of integration points increases [6,9,11].

Symplectic integrators can be derived by a variety of ways [12,13]. Early investigators, guided by Hamilton–Jacobi theory, constructed symplectic integrators from generating functions which approximately solve the Hamilton–Jacobi equation [2,4,7]. Moreover, the symplectic splitting technique is based on the property that symplectic integrators form a group, and thus, the composition of symplectic-preserving maps is also symplectic. Here the idea is to split the Hamiltonian

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into terms whose flow can be explicitly solved and then compose these individual flows in such a way that the resulting (composite) flow is consistent with the Hamiltonian flow [5].

On the other hand, variational integration techniques determine integrators from a discrete Lagrangian and the associated discrete variational principle [9,14–16]. The discrete Lagrangian can be designed to inherit the symmetry associated with the action of a Lie group, and, hence by a discrete Noether's theorem these methods can also preserve momentum invariants. For an extended discussion of the above statements, see Refs. [1,17,18].

In the present work, we propose a new approach for the construction of variational integrators based on the fact that only the partial derivatives of the action integral of the Lagrangian are needed in the general theory. The analytic calculation of these derivatives, creates a new integral that depends not on the Lagrangian itself, but on the Euler–Lagrange vector, which in the continuous and exact case vanishes. Since this new integral can only be computed through a numerical method relying on some internal grid points, we can locally fit the exact curve by demanding the Euler–Lagrange vector to vanish at these grid points. In this way, the integral vanishes, and the process tremendously simplifies the calculation of high order approximations.

In the rest of the paper, at first (Section 2), the main characteristics of the discrete variational integrators are briefly outlined and the formalism of the local path fitting method is presented (Section 3). Then, an application of the new method and its role to the harmonic oscillator and to orbital problems with ultra high eccentricity ($\epsilon = 0.99$) is addressed (Section 4). The benefits of the improved integrator are demonstrated in the numerical solutions of the 2-body problem and the mechanical system of five outer planets (Section 5). Finally the main conclusions coming out of the present work are briefly summarized (Section 6).

2. Discrete variational mechanics

Within the context of the variational integration theory, one derives integrators for mechanical systems coming out of the discrete variational principles [6,9,14,19]. Variational principles have been successfully applied to partial differential equations and to stochastic systems as well. In the general theory, discrete analogs of the continuous Lagrangian, Euler–Lagrange equations, Hamilton's principle, Noether's theorem, and Legendre transform can be rather easily obtained (see e.g. Refs. [9,20]). Moreover, variational integrators can readily incorporate holonomic constraints (through the use of Lagrange multipliers) and non-conservative effects (via their virtual work) [9,14].

Recently, variational principles have been applied to particle mesh methods and to fractional stochastic optimal control problems [21–23]. The algorithms derived from these discrete principles have been successfully tested in infinite and finite-dimensional conservative, dissipative, smooth and non-smooth mechanical systems (see e.g. Refs. [15,16] and the references therein).

In the general approach, the relevant variational principle creates an estimation of the action integral in a time interval $[t_0, t_1]$ as a smooth function of the edges of a segment of the system's trajectory (q_0, q_1). Since any sufficiently smooth and non-degenerate function $S(q_0, q_1)$ generates, via

$$p_0 = -\frac{\partial S(q_0, q_1)}{\partial q_0}$$
$$p_1 = \frac{\partial S(q_0, q_1)}{\partial q_1},$$

a symplectic map $(q_0, p_0) \rightarrow (q_1, p_1)$ [24], the estimated action integral can be used to develop a discrete analog to the continuous Euler–Lagrange equations as it is briefly outlined below.

The well known least action principle of the continuous Lagrange–Hamilton dynamics can be used as a guiding principle to derive discrete integrators, [9,14,20]. For this purpose, one considers the positions q_0 and q_1 and a time step $h \in R$ ($h = t_1 - t_0$), in order to replace the parameters of position q and velocity $\dot{q}$ in the continuous time Lagrangian $L(q, \dot{q}, t)$. Then, by taking the variable h as a very small (positive) number, the positions q_0 and q_1 could be assumed as being two points on a curve (trajectory of the mechanical system) at time h apart. Under these assumptions, the following approximations hold

$$q_0 \approx q(0), \qquad q_1 \approx q(h),$$

and a function $L_d(q_0, q_1, h)$, known as discrete Lagrangian, is defined to approximate the action integral along the curve segment with endpoints q_0 and q_1, as

$$L_d(q_0, q_1, h) = \int_0^h L(q, \dot{q}, t)dt. \tag{1}$$

Furthermore, one may consider the very simple approximation for this integral given on the basis of the rectangle rule [9] according to which $\int_0^h L dt \approx hL$, where the value of L is obtained by replacing the velocity $\dot{q}$ with the approximation $(q_1 - q_0)/h$.

The next step is, by considering the discrete curve defined by the set of points $\{q_k\}_{k=0}^{N}$, to calculate the discrete action sum S_d along this sequence of segments, $[q_k, q_{k+1}]$, $k = 0, 1, \ldots, N-1$, by summing the discrete Lagrangians of the form $L_d(q_k, q_{k+1}, h)$ defined for each adjacent pairs of points (q_k, q_{k+1}), as

$$S_d(\gamma_d) = \sum_{k=1}^{N} L_d(q_{k-1}, q_k), \quad \gamma_d = (q_0, \ldots, q_{N-1}) \in Q^n \tag{2}$$

where γ_d is a discrete trajectory of the mechanical system. The discrete Hamilton's principle states that, γ_d extremizes the action sum, i.e., $\delta S_d(\gamma_d) = 0$. By carrying out the differentiation and rearrangement of the terms in the latter equation, keeping in mind that the endpoints q_0 and q_N are fixed, the discrete Euler–Lagrange (DEL) equations are obtained:

$$D_2L_d(q_{k-1}, q_k, h) + D_1L_d(q_k, q_{k+1}, h) = 0 \tag{3}$$

where the notation D_iL_d denotes the slot derivative with respect to the i-th argument of L_d.

From a geometrical point of view, for the discrete Lagrangian L_d we have $L_d : Q \times Q \to R$, where Q is the space of generalized positions q. Hence, in the discrete setting the corresponding space for the velocity (phase space TQ) is $Q \times Q$. An intuitive motivation for this is that two points close to each other correspond approximately to the same information as one point and a velocity vector [9].

We can define now the map $\Phi : Q \times Q \to Q \times Q$, by

$$D_1L_d \circ \Phi + D_2L_d = 0 \tag{4}$$

which means that $\Phi(q_{k-1}, q_k) = (q_k, q_{k+1})$. Hence, if for each $q \in Q$, the map $D_1L_d(q, q) : T_qQ \to T_q^*Q$ is invertible, then $D_1L_d : Q \times Q \to T^*Q$ is locally invertible and so the discrete flow defined by the map Φ is well defined for small enough time steps (see Ref. [17] for details). Moreover, we define the known as fiber derivative

$$F_{L_d} : Q \times Q \to T^*Q \tag{5}$$

and the two-form ω on $Q \times Q$ by pulling back the canonical two-form $\Omega_{CAN} = dq^i \wedge dp^i$ from T^*Q to $Q \times Q$, by the expression

$$\omega = {F_{L_d}}^*(\Omega_{CAN}). \tag{6}$$

The coordinate expression for ω is

$$\omega = \frac{\partial^2 L_d(q_k, q_{k+1})}{\partial q_k^i \partial q_{k+1}^j} dq_k^i \wedge dq_{k+1}^j \tag{7}$$

and it can be easily proved that the map Φ preserves the symplectic form of ω (two different proofs are presented in Refs. [14,18]). Finally, assuming that the discrete Lagrangian is invariant under the action of a Lie group G on Q and in its cotangent space $\xi \in g$ defined in the Lie algebra of G, by analogy with the continuous case, we can construct the discrete momentum map $J_d : Q \times Q \to g^*$ by

$$\langle J_d(q_k, q_{k+1}), \xi \rangle := \left\langle D_a L_d(q_k, q_{k+1}), \xi_Q(q_k) \right\rangle. \tag{8}$$

As can be proved, the map Φ preserves the momentum map J_d; see e.g. Refs. [14,17].

In a position-momentum representation, the discrete Euler–Lagrange equations (3) can be written in the form [9]

$$\begin{aligned} p_k &= -D_1L_d(q_k, q_{k+1}, h) \\ p_{k+1} &= D_2L_d(q_k, q_{k+1}, h). \end{aligned} \tag{9}$$

In the next section, a new variational integrator is proposed that is inspired by the fact that only the partial derivatives of the discrete Lagrangian are needed in the latter equations. The calculation of these derivatives, provides a new integral that depends on the Euler–Lagrange vector itself, which vanishes in the continuous and exact case.

3. The new approach of local path fitting

The new method based on the variational integrators theory arises from the system of differential equations (9), which can be considered as a numerical one-step procedure $(q_k, p_k) \to (q_{k+1}, p_{k+1})$. In general, the level of the accuracy in the estimation of the action integral

$$L_d(q_k, q_{k+1}, h) \sim \int_{t_k}^{t_{k+1}} L(q, \dot{q}, t)dt \tag{10}$$

characterizes the accuracy of the resulting method [16].

From Eqs. (9), one can imply that only the derivatives of the discrete Lagrangian L_d are needed to be calculated. For obtaining these derivatives, we consider a free parameter λ which, in general, may enter q, $\dot{q}$ and h. Then, obviously, we have

$$\frac{\partial L_d(q_k, q_{k+1}, h)}{\partial \lambda} = L(q(t_{k+1}), \dot{q}(t_{k+1}), h)\frac{\partial h}{\partial \lambda} + \int_{t_k}^{t_{k+1}} \frac{\partial L(q, \dot{q}, t)}{\partial \lambda} dt. \tag{11}$$

By using the rules of differentiation

$$\frac{\partial L(q, \dot{q}, t)}{\partial \lambda} = \frac{\partial L(q, \dot{q}, t)}{\partial q}\frac{\partial q}{\partial \lambda} + \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\frac{\partial \dot{q}}{\partial \lambda} \tag{12}$$

and changing the order of derivation in the second term of the right hand side (r.h.s.) of the above equation we get

$$\frac{\partial L(q, \dot{q}, t)}{\partial \lambda} = \frac{\partial L(q, \dot{q}, t)}{\partial q}\frac{\partial q}{\partial \lambda} + \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\frac{d\frac{\partial q}{\partial \lambda}}{dt}. \tag{13}$$

Inserting the latter equation in Eq. (11) and integrating by parts gives

$$\begin{aligned}\frac{\partial L_d(q_k, q_{k+1}, h)}{\partial \lambda} &= L(q(t_{k+1}), \dot{q}(t_{k+1}), h)\frac{\partial h}{\partial \lambda} \\ &\quad + \int_{t_k}^{t_{k+1}} \left(\frac{\partial L(q, \dot{q}, t)}{\partial q} - \frac{d}{dt}\left(\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\right)\right)\frac{\partial q}{\partial \lambda} dt + h\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\frac{\partial q}{\partial \lambda}\Big|_{t_k}^{t_{k+1}}.\end{aligned} \tag{14}$$

It is now clear that instead of estimating the integral in Eq. (10) using any quadrature rule based on a set of $S+1$ grid points at times $\{t_k + c^j h,\ j = 0, 1, \ldots, S\}$, with $c^0 = 0$ and $c^S = 1$, we only have to estimate the integral

$$I_0 = \int_{t_k}^{t_{k+1}} \left(\frac{\partial L(q, \dot{q}, t)}{\partial q} - \frac{d}{dt}\left(\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\right)\right)\frac{\partial q}{\partial \lambda} dt. \tag{15}$$

On the other hand, if we demand fulfillment of the Euler–Lagrange equation,

$$\frac{\partial L(q, \dot{q}, t)}{\partial q} - \frac{d}{dt}\left(\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\right) = 0, \tag{16}$$

at these grid points, we get $I_0 = 0$ and subsequently

$$\frac{\partial L_d(q_k, q_{k+1}, h)}{\partial \lambda} = L(q(t_{k+1}), \dot{q}(t_{k+1}), h)\frac{\partial h}{\partial \lambda} + h\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\frac{\partial q}{\partial \lambda}\Big|_{t_k}^{t_{k+1}}. \tag{17}$$

The set of Eqs. (9) are then written as

$$\begin{aligned} p_k &= -\frac{\partial L_d(q_k, q_{k+1}, t)}{\partial \dot{q}}\frac{\partial q}{\partial q_k} \\ p_{k+1} &= \frac{\partial L(q_k, q_{k+1}, t)}{\partial \dot{q}}\frac{\partial q}{\partial q_{k+1}}. \end{aligned} \tag{18}$$

The above set of equations is consistent with the variational principles.

If we consider the $S+1$ grid points, $q^j,\ j = 0, 1, \ldots, S$, at times $t^j = t_k + c^j h$, with $c^0 = 0$ and $c^S = 1$ at the edge points $q_k,\ q_{k+1}$, for these internal points we have

$$\frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}\frac{\partial q}{\partial q^j}\Big|_{t_k}^{t_{k+1}} = 0, \quad j = 1, 2, \ldots, S-1. \tag{19}$$

Also for the internal points q^j of the segment with endpoints q_k and q_{k+1}, we have

$$\frac{\partial L_d}{\partial q^j} = 0 \tag{20}$$

as the curve is fixed at its endpoints. Eqs. (18)–(20) summarize the main formalism of the new local path fitting method which we test in the following mechanical systems.

3.1. Solving the harmonic oscillator using local path fitting

For a first test, the proposed method is applied to the well known problem of the harmonic oscillator with unity frequency that is described by the Lagrangian

$$L = \frac{1}{2}\dot{q}^2 - \frac{1}{2}q^2. \tag{21}$$

To obtain the oscillations we can calculate $q(t)$ with t in the interval $t \in [0, h]$ with $h = t_{k+1} - t_k$, by the following expression

$$q(t) = \left(1 - \frac{t}{h}\right) q_k + \left(\frac{t}{h}\right)\left(1 - \frac{t}{h}\right) x_1 + \left(\frac{t}{h}\right)^2 \left(1 - \frac{t}{h}\right) x_2 + \left(\frac{t}{h}\right) q_{k+1} \tag{22}$$

where x_1, x_2 are free parameters (coefficients) to be calculated which play the same role as the parameter λ in the previous formalism.

The approximation of Eq. (22) has been defined in such a way that at $t = t_k = 0$ and $t = t_{k+1} = h$ to give the endpoints q_k and q_{k+1}, respectively. By demanding that the Euler–Lagrange equations hold at the endpoints, any quadrature rule for the calculation of the action integral, based on the edge points of the curve, will give the set of Eq. (18).

In order to generalize Eq. (22), we define

$$\tau = \frac{t - t_k}{h}, \quad \tau \in [0, 1]$$
$$t = t_k + \tau h, \quad t \in [t_k, t_{k+1}];$$

then Eq. (22) is written as

$$q(t) = (1 - \tau)q_k + \tau(1 - \tau)x_1 + \tau^2(1 - \tau)x_2 + \tau q_{k+1}. \tag{23}$$

Calculating the derivations of the above equation we obtain

$$\dot{q}(t) = \frac{dq}{d\tau}\frac{d\tau}{dt} = -\frac{1}{h}q_k + \frac{1}{h}(1 - 2\tau)x_1 + \frac{1}{h}(2\tau - 3\tau^2)x_2 + \frac{1}{h}q_{k+1}$$
$$\ddot{q}(t) = -\frac{2}{h^2}x_1 + \frac{1}{h^2}(2 - 6\tau)x_2.$$

The parameters x_1, x_2 of Eqs. (22)–(23) can now be easily calculated by demanding that the discrete Euler–Lagrange equations hold. So we obtain

$$x_1 = \frac{h^2}{3}\left(q_k + \frac{q_{k+1}}{2}\right)$$
$$x_2 = \frac{h^2}{6}(q_{k+1} - q_k).$$

The proposed method then gives

$$q_{k+1} = \frac{6h\dot{q}_k + q_k(6 - 2h^2)}{6 + h^2}$$
$$\dot{q}_{k+1} = \frac{q_{k+1} - q_k}{h} - \frac{h}{3}\left(q_k + \frac{q_{k+1}}{2}\right).$$

Fig. 1 shows the exact orbit $q(t)$ and the positions q_k calculated by using the local path fitted method for the case where $q(t)$ is described from Eq. (22). It is clearly shown that the two orbits are identical. The results have been taken for the first 10 periods using a time step $h = 0.01$ with unity frequency ($\omega = 1$).

4. Local path fitting using Bernstein basis polynomials

For a better approximation of the discrete trajectory $q(t)$ described above, we introduce the Bernstein basis polynomials which have been defined in Ref. [25] and have the advantage to approximate a continuous function [25–28]. Here we will employ them to write Eq. (22) in a more compact and convenient form.

The $n + 1$ Bernstein basis polynomials of degree n are defined as

$$b_{j,n}(\tau) = \binom{n}{j} \tau^j (1 - \tau)^{n-j}, \quad j = 0, 1, \ldots, n \tag{24}$$

($\tau \in [0, 1]$) where $\binom{n}{j}$ is the known binomial coefficient (see Appendix). The basic properties of these polynomials, which are required for the purposes of the present work, are summarized in Appendix.

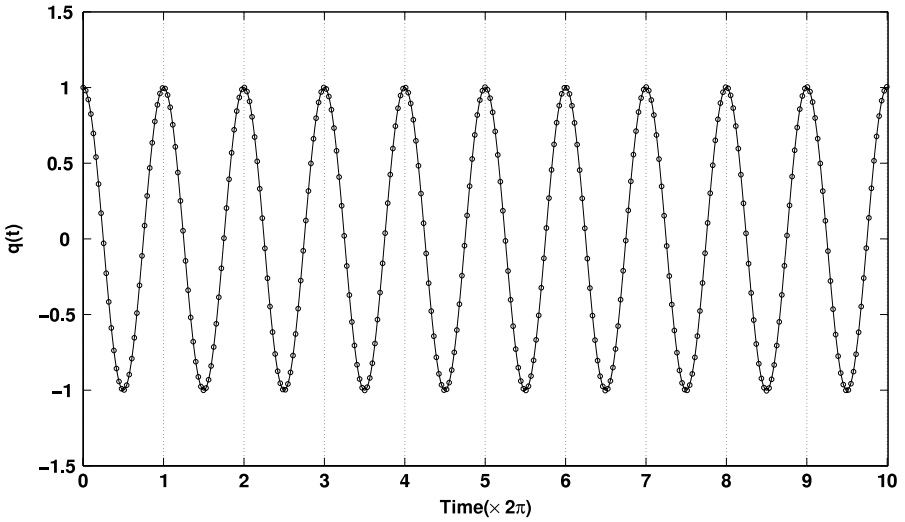

Fig. 1. The exact orbit (solid line) for the harmonic oscillator with unity frequency ($\omega = 1$) and the calculated (using the local path fitted method) points (○) for the first 10 periods. An orbit satisfying the Euler–Lagrange equation at the edge points has been employed.

We then consider the Lagrangian $L(q, \dot{q}, t)$ of a given system and the state vector (q_k, p_k) at a given time t_k. By assuming $x^j,\ j = 0, 1, \ldots, S$ to be a set of $S + 1$ parameters defined on the grid points, we define $q(t)$ through the polynomial form

$$q(t) = \sum_{j=0}^{S} x^j b_{j,S}(\tau), \quad t \in [t_k, t_{k+1}] \tag{25}$$

with

$$\tau = \frac{t - t_k}{h}, \quad 0 \le \tau \le 1 \tag{26}$$

($h = t_{k+1} - t_k$). Eq. (25) represents the analog of Eq. (23) in Bernstein basis polynomial and gives the position q at a time $t \in [t_k, t_{k+1}]$ (here we do not put $t_k = 0,\ t_{k+1} = h$ as in the previous example). This equation expresses the fact that x^j are the so called Bernstein coefficients (Bézier coefficients).

Since $q(t_k) = x^0$ and $q(t_{k+1}) = x^S$, from Eq. (25) we have

$$q(t) = q_k b_{0,S}(\tau) + \sum_{j=1}^{S-1} x^j b_{j,S}(\tau) + q_{k+1} b_{S,S}(\tau). \tag{27}$$

Replacing the position $q(t)$ and velocity $\dot{q}(t)$ in the Lagrangian and demanding satisfaction of the Euler–Lagrange equation (9) in the grid points, we get

$$\begin{aligned} p_k &= -\left.\frac{\partial L}{\partial \dot{q}}\right|_{t=t_k} \\ &\left.\frac{\partial L}{\partial q}\right|_{t=t_k+c^j h} - \frac{d}{dt}\left(\left.\frac{\partial L}{\partial \dot{q}}\right)\right|_{t=t_k+c^j h} = 0, \quad j = 1, 2, \ldots, S-1 \\ p_{k+1} &= \left.\frac{\partial L}{\partial \dot{q}}\right|_{t=t_{k+1}}. \end{aligned} \tag{28}$$

By solving the above system for $x^j,\ j = 0, 1, 2, \ldots, S-1$ and p_{k+1}, the next points $q_{k+1} = x^S$ can be calculated during a typical one step procedure.

5. Numerical tests

As some concrete applications of the above method we explore its efficiency and the integration steps needed to obtain small energy error in the two body problem and the five outer planets relative to the Sun in our solar system [29].

5.1. The 2-body problem

We first study the problem of two objects mutually interacted through a central force. The most famous example of this type is the Kepler's problem (also called the two body problem) that describes the motion of two bodies which attract

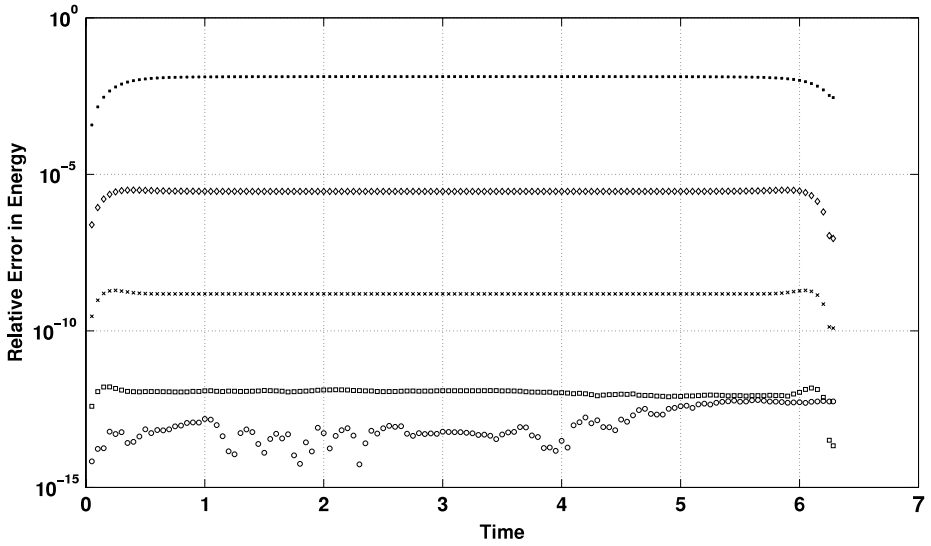

Fig. 2. The relative error in energy during one period for eccentricity $\epsilon = 0.5$, step size $h = 0.05$ and for different values of S (number of intermediate points). (■) for $S = 3$, (◇) for $S = 5$, (×) for $S = 7$, (□) for $S = 9$ and (○) $S = 11$.

Table 1
Number of integration steps.

S	3	4	5	6	7	8	9	10	11	12
No of steps	$> 10^4$	$> 10^4$	3526	460	421	181	142	112	98	59

Table 2
Comparison of the number of integration steps needed for one period in the two body problem to obtain energy error 10^{-6} with eccentricity $e = 0.95$, in various methods (see text).

Order	Linear [9]	Local path	EMB5 [30]
5	3245	790	1182
6	2453	580	

each other with a central force (its direction is in the line connecting their centers). In the solar system the gravitational interaction between two bodies leads to the elliptic orbits of planets and the hyperbolic orbits of comets.

By choosing one of the bodies (the heavier) as the center of our coordinate system, the motion will remain planner. Denoting the position of the second body by $\mathbf{q} = (q_1, q_2)^T$, the Lagrangian of the system (assuming the masses of the bodies and the gravitational constant equal to 1) takes the form

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{1}{2}\dot{\mathbf{q}}^T\dot{\mathbf{q}} + \frac{1}{|\mathbf{q}|}. \tag{29}$$

As initial conditions (position and velocity) we assume

$$\mathbf{q} = (1-\epsilon, 0)^T, \qquad \dot{\mathbf{q}} = \left(0, \sqrt{\frac{1+\epsilon}{1-\epsilon}}\right)^T \tag{30}$$

where ϵ is the eccentricity of the orbit.

In the first computational experiment, we take the eccentricity $\epsilon = 0.5$ and the time step $h = 0.05$ and plot the relative error in the energy during one period for several numbers of intermediate points S. The results are shown in Fig. 2 from which it is clear that the order of the approximation is increased with increasing the number of intermediate points.

In the second simulation experiment, we take the eccentricity $\epsilon = 0.99$ and use an adaptive time step control in order to keep the relative error in energy smaller than 10^{-7}. Table 1 shows the number of integration steps needed for one period in several cases of intermediate points. As can be seen, the order of approximation is clearly increased with increasing S as, the mean time step needed for the same error in energy increases from $1.8 \cdot 10^{-3}$ for $S = 5$–0.1 for $S = 12$.

In Table 2, the linear method (second column) corresponds to the variational integrator described in Ref. [9]. In the fourth column (labeled 'EMB5'), the results have been obtained with the embedded 5th order exponential fitted method of Ref. [30].

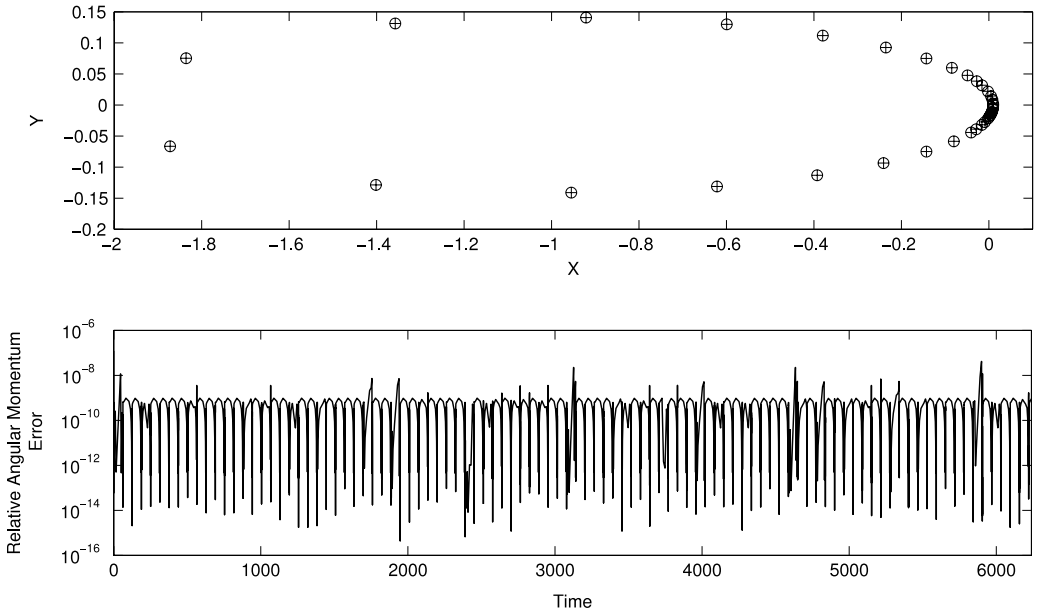

Fig. 3. Long term integration of the 2-body problem with eccentricity $\epsilon = 0.99$ for 10^3 periods with $S = 12$ intermediate points and a time step which is adaptively calculated in order to keep the relative error in energy less than 10^{-7}. In the first (top) plot, the calculated (+) and the exact (∘) positions of the orbiting body are plotted for the last period. In the second (bottom) plot, the relative error in the angular momentum is plotted.

By comparing the local path fitted method with the linear one [9], we conclude that in the proposed technique the time step needed to achieve the same error in energy is larger. As a result, the number of integration steps needed for one period, is 4 times less for the fifth order and 5 times less for the case of sixth order compared to the linear method. This is a remarkable result illustrating the better behavior of the local path fitted technique. The number of steps of our method in the case of the 5th order appears to be much smaller to those required by the EMB5 method [30].

In Fig. 4, the efficiency of the proposed method is illustrated by plotting the counting calculation time (CPU time) versus energy error and comparing it with that of the phase-fitted discrete Lagrangian method presented in [23]. As expected, the smaller the error the larger the CPU time is shown in both methods. It is clear, however, that the present method is appreciably more accurate than the phase fitted method especially for smaller errors, e.g. for energy error 10^{-5} the CPU time of the local path method is about four times smaller, namely more efficient of that in [23].

Finally, in the last experiment we integrate the two-body problem with eccentricity $\epsilon = 0.99$ for 10^4 periods in order to check the long term behavior of the method. The number of intermediate points is $S = 12$ and the time step is adaptively controlled in order to keep the relative error in energy less than 10^{-7}. The results for the position q_k of the body's orbit (calculated with the proposed method and exact ones) and the relative error in angular momentum, are demonstrated in Fig. 3. In the upper sub-figure, we plot the positions (of the lighter body) during the last period of the motion along with the exact solution, while in the bottom sub-figure, the relative error in angular momentum is illustrated.

In both cases, the results demonstrate the excellent behavior of the method, even for orbits with extremely high eccentricity and for very large number of periods. As can be seen, when $S = 12$ intermediate points are chosen and use of an adaptive time step is made, the number of steps needed to obtain the orbital motion (although from Table 1 it looks as a rather small number) are enough to preserve the symplectic structure of the method. Even more, the relative angular momentum error is less than 10^{-9} and the same behavior is kept even after a very high number of periods. This can be considered as a good advantage of our method.

5.2. The 5-outer planets system

The next problem we have chosen for numerical computation with our new method concerns with the motion of the five outer planets relative to the Sun. The problem falls in the category of the N-Body problem related to the motion of N bodies under Newton's law of gravity. The Lagrangian of this system reads

$$L(q, \dot{q}, t) = \frac{1}{2}\sum_{i=0}^{N} m^i \left(\dot{q}^i\right)^T \dot{q}^i + G\sum_{j=1}^{N}\sum_{k=0}^{j-1} \frac{m^j \cdot m^k}{\|q^j - q^k\|} \tag{31}$$

where G is the gravitational constant, m^i, q^i and $\dot{q}^i$ are the mass, the position vector and the velocity vector, respectively, of the i-th body.

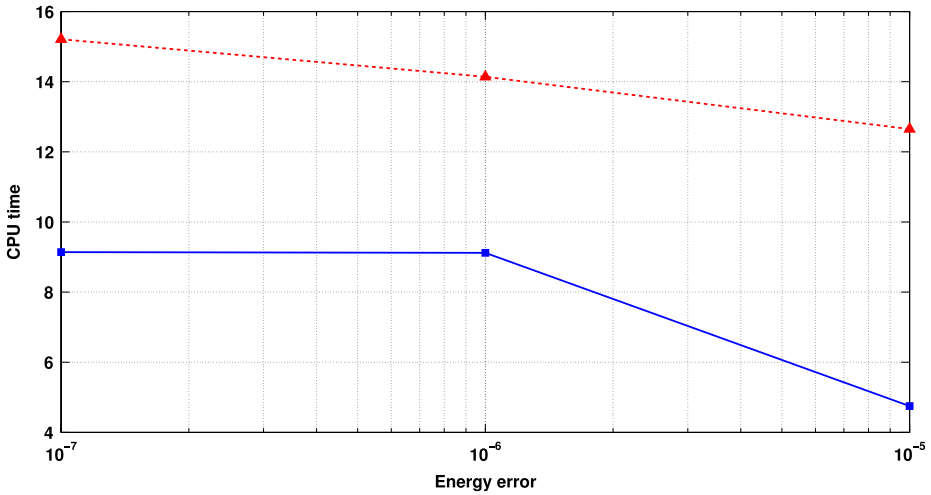

Fig. 4. The CPU time (in arbitrary units) needed for the proposed method (continuous line) and the Phase fitted discrete Lagrangian method (dashed line) of Ref. [23]. Both methods are of 5th order and are applied in the two body problem for eccentricity $e = 0.6$ for one period.

Table 3
Initial data for the 5-outer planet problem in our solar system.

Planet	Mass	Initial position	Initial velocity
Sun	1.00000597682	0	0
		0	0
		0	0
Jupiter	0.000954786104043	−3.5023653	0.00565429
		−3.8169847	−0.00412490
		−1.5507963	−0.00190589
Saturn	0.000285583733151	9.0755314	0.00168318
		−3.0458353	0.00483525
		−1.6483708	0.00192462
Uranus	0.0000437273164546	8.3101420	0.00354178
		−16.2901086	0.00137102
		−7.2521278	0.00055029
Neptune	0.0000517759138449	11.4707666	0.00288930
		−25.7294829	0.00114527
		−10.8169456	0.00039677
Pluto	$1/(1.3 \cdot 10^8)$	−15.5387357	0.00276725
		−25.2225594	−0.00170702
		−3.1902382	−0.00136504

In Ref. [24], the data for the five outer planets problem is given. The necessary data for the purposes of the present work are summarized in Table 3. Masses are relative to the Sun, so that the Sun has mass 1. In the computational calculations, the Sun with the four inner planets are considered as one body, so its mass is larger than one. Distances are in astronomical units, time is in Earth days and the gravitational constant is $G = 2.95912208286 \cdot 10^{-4}$.

The Lagrangian of Eq. (31) has been integrated for $t \in [0, 10^6]$ days, with a time step $h = 50$ days and using $S = 6$ intermediate points. The results are shown in Fig. 5. The planet orbits are obtained stable, the maximum relative error in energy is $\sim 10^{-7}$, the maximum relative error in momentum is less than 10^{-10} and finally the relative error in angular momentum is $\sim 10^{-9}$.

We note that, the errors in angular momentum are mostly due to the round off error produced by the solution of the non-linear system used to calculate the intermediate points.

From Fig. 5, it becomes obvious that the main advantages of the proposed integrator arise from the symplectic behavior of the method. The local path fitted method, when used for multi body problems, as the outer planets problem, and for high number of periods (in our case 10^6 days), preserve the symplectic structure of the problem, described from system's angular momentum. Even more, the Bernstein basis polynomials (used for the interpolation of the intermediate points) when combined with the perspective to keep the relative energy error rather small (a quantity which can be changed by the user), force the bodies to keep their orbits. At the end, the calculated relative error in momentum from the proposed algorithm is less than 10^{-11}. This is also a remarkable result since, even after an extremely high number of periods (hundred thousand of days) the error in momentum is less than 10^{-13}.

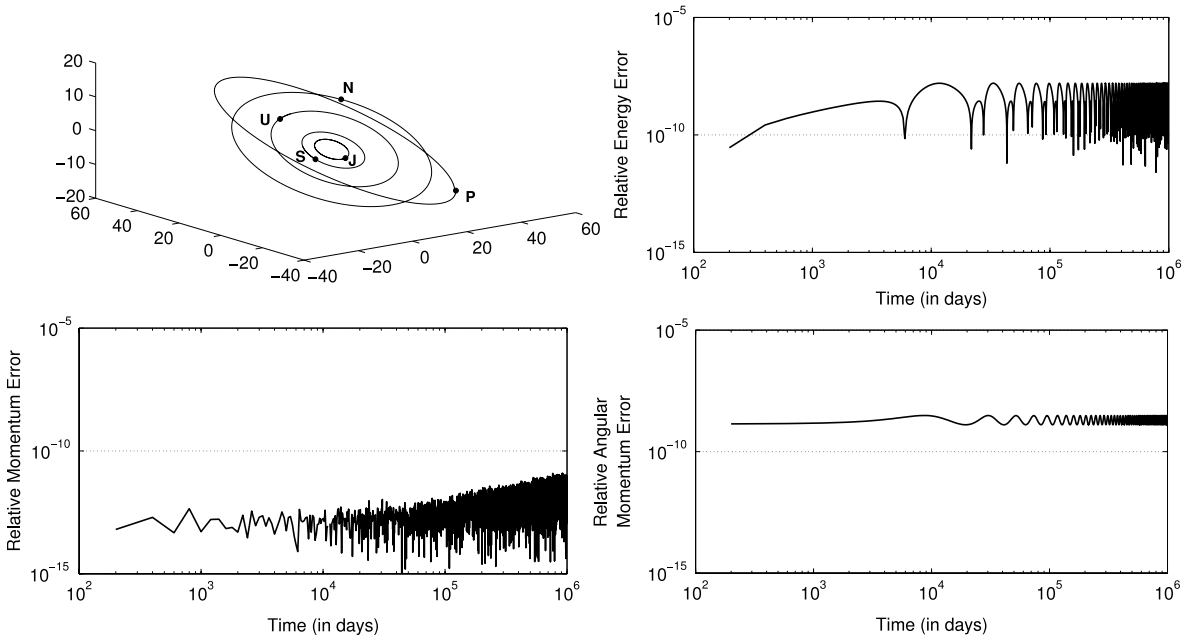

Fig. 5. Integration of the outer solar system for 10^6 days with time step $h = 50$ days and $S = 6$ intermediate points. The planets (Jupiter, Saturn, Uranus, Neptune and Pluto) follow constant orbits, while the relative error in energy is $\sim 10^{-7}$, the maximum relative error in momentum is less than 10^{-10} and, finally, the relative error in angular momentum is $\sim 10^{-9}$.

Before closing we note that, in generally, the accuracy is not the primary advantage of the application of variational integrators, but rather their ability to discretely preserve essential structure of a continuous system and to compute statistical properties of larger groups of orbits, such as Poincaré sections or temperature of a system (see, for example, Refs. [16,31]).

On the other hand, high accuracy can be obtained using specially designed methods as it is explained in Refs. [23,32]. Even though these methods produce high order estimations of the positions and the momenta, computationally become very heavy as the order increases. This is due to the large number of parameters that have to be calculated in each step (depending on the nature of the Lagrangian) as a solution to a non-linear system. The entire set of equations, consists of partial derivatives of the action integral and a set of variational equations that determine the internal points, needed for high order methods (see also Ref. [29]).

6. Summary and conclusions

In the present work, a new approach for constructing variational integrators has been developed. This new technique is based on the fact that, the construction of the symplectic map in the variational integrator, needs only the estimation of the partial derivatives of the action integral in a time interval. These derivatives in the proposed method are functions of the integral of the Euler–Lagrange vector, which in the exact case vanishes.

Thus, taking an orbit which satisfies the Euler–Lagrange equation in a number of grid points, any quadrature used for the calculation of the action integral vanishes and the process is significantly simplified.

Experimental tests show that this method efficiently integrates stiff systems (like the two body problem with eccentricity up to 0.99) conserving all the benefits of the classical variational integrators.

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Appendix. Bernstein basis polynomials

The Bernstein basis polynomials are defined as

$$b_{j,n}(\tau) = \binom{n}{j} \tau^j (1-\tau)^{n-j}, \quad j = 0, 1, \ldots, n \tag{A.1}$$

and described the Bernstein polynomial

$$B(\tau) = \sum_{j=0}^{n} x^j b_{j,n}(\tau) \tag{A.2}$$

where $\binom{n}{j}$ is the known binomial coefficient defined as

$$\binom{n}{j} = \frac{n!}{j!(n-j)!}. \tag{A.3}$$

The main properties of the Bernstein basis polynomials are summarized in the equations below

$$b_{j,n}(0) = \delta_{j0}$$
$$b_{j,n}(1) = \delta_{jn}$$

with δ being the Kronecker delta symbol.

If $n \neq 0$, then $b_{j,n}(\tau)$ has a unique local maximum on the interval [0, 1] at $\tau = \frac{j}{n}$. This maximum takes the value

$$j^j n^{-n} (n-j)^{n-j} \binom{n}{j}. \tag{A.4}$$

For other properties see Refs. [25–28].

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