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Variational Integrators for Higher Order Lagrangians

by
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Abstract

We study conservative numerical methods for the Euler-Lagrange equations when the lagrangian is $Lag{=}L\left(y, y', y'', ..y^{(k)}\right)dx$

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1 Preliminaries

Let consider the fibration of $\pi_{XY} : Y \rightarrow X$ where X is the real field and the fibers are diffeomorphic to a given finite dimensional manifold Q. A k jet over $x \in X$ is a class of equivalence of sections of Y defined in a neighborhood of x such that two sections are equivalent iff their Taylor development agree up to order k. The jet corresponding to section s will be denoted by $j^k s(x)$. The definition is independent of the local coordinates on X or Q. If x is a local coordinate on X and $\left(y^1,\ y^2,\ ..y^N\right)$ are local coordinates on Q, then on J^kY we use the coordinates $\left(x, y^A, y_i^A\right)_{A=1..A,\ i=1..k}$, where for the jet of a section $s : X \rightarrow Y$, $s(x) = \left(x, s^1(x), s^2(x), ..s^N(x)\right)$ we have $y^A = s^A(x)$, $y_i^A = \frac{d^i}{dx^i}s^A(x)$. In the following y_0^A is identical to y^A. The correspondence $x \rightarrow j^k s(x)$ is a section of J^kY and is denoted by $j^k s$. By truncation of a k development to a l development (l<k) we get a projection $\pi_{J^lY,J^kY} : J^kY \rightarrow J^lY$.

Using local coordinates we define the total derivative $D_x = \frac{\partial}{\partial x} + y_1^A\frac{\partial}{\partial y^A} + y_2^A\frac{\partial}{\partial y_1^A} + ... + y_k^A\frac{\partial}{\partial y_{k-1}^A} + y_{k+1}^A\frac{\partial}{\partial y_k^A}$ as a function from $J^{k+1}Y$ to the tangent space TJ^kY and we define also the differential forms $\theta_0^A = \theta^A = dy^A - y_1^A dx$, $\theta_j^A = dy_j^A - y_{j+1}^A dx$, for $j \geq 1$. For any section s we have $j^k s^*\left(\theta_j^A\right) = 0$, and $\theta_j^A(D_x) = 0$. By lagrangian on J^kY we understand a differential form of degree 1 which to any jet $\gamma \in J^kY$ takes value in $\pi^*_{X,J^kY}\left(\Lambda^1 X\right)$. Using local coordinates, a lagrangian is a differential form

$$Lag{=}L\left(x, y^A, y_1^A, ..y_k^A\right) dx \tag{1}$$

Any function $f : J^kY \to R$ can be considered as a function denoted abusively f also, defined on any J^nY (n>k) by the composition $J^nY \overset{\pi_{J^kY,J^nY}}{\to} J^kY \overset{f}{\to} R$. Analogously any form $\omega \in \Lambda J^kY$ gives a form on J^nY (n>k) by the formula $\pi^*_{J^kY,J^nY}\omega$. For such functions D_xf is well defined on an open set of $J^{k+1}Y$. We define $D_{x,p} = D_x \circ D_x \circ ..D_x$ (p times) which gives for $f : J^kY \to R$, a function $D_{x,p}f : J^{k+p}Y \to R$, by the formula $D_{x,p}f = D_xD_x\left(..D_x\left(f\right)\right)$. For p=0 we define $D_{x,0}$ =identity. For a section s of Y we have

$$\frac{d}{dx}\left(f\left(x, s^A\left(x\right), \frac{ds^A\left(x\right)}{dx}, ..\frac{d^ks^A\left(x\right)}{dx^k}\right)\right)$$
$$= \left(D_xf\right)\left(x, s^A\left(x\right), \frac{ds^A\left(x\right)}{dx}, ..\frac{d^ks^A\left(x\right)}{dx^k}, \frac{d^{k+1}s^A\left(x\right)}{dx^{k+1}}\right) = \left(D_xf\right)\left(j^{k+1}s\left(x\right)\right)$$

We have the following result:

Proposition 1. *Let Lag a lagrangian defined on* J^kY*. Then the following form*

$$\theta_{Lag} = Ldx + \sum_{A=1}^{N}\sum_{j=1}^{k}\sum_{m=0}^{j-1}\left(-1\right)^m D_{x,m}\frac{\partial L}{\partial y_j^A}\cdot\theta^A_{j-m-1} \tag{2}$$

$$= Ldx + \sum_{A=1}^{N}\sum_{b=0}^{k-1}\sum_{m=0}^{k-b-1}\left(-1\right)^m D_{x,m}\frac{\partial L}{\partial y^A_{m+b+1}}\cdot\theta^A_b \tag{3}$$

is well defined on $J^{2k-1}Y$ *(independent of the coordinate system).*

For a proof see [15].

□

Now let s^ε a C^∞ family of sections $s^\varepsilon : \left[a\left(\varepsilon\right), b\left(\varepsilon\right)\right] \to Y$ defined for ε in a neighborhood of 0, let j^ks^ε the k jet of s^ε and let $\zeta = \frac{d}{d\varepsilon}|_{\varepsilon=0}s^\varepsilon$. We shall denote s^0 simply s. An integration by parts gives

$$\frac{d}{d\varepsilon}|_{\varepsilon=0}\int_{a(e)}^{b(\varepsilon)} L\left(j^ks^\varepsilon\left(x\right)\right)dx = \sum_{A=1}^{N}\sum_{j=0}^{k}\int_a^b\left(-1\right)^j D_{x.j}\frac{\partial L}{\partial y_j^A}\left(j^{2k}s\left(x\right)\right)\cdot\zeta^A\left(x\right)dx$$
$$+ L\left(j^ks\left(b\right)\right)b'\left(0\right) - L\left(j^ks\left(a\right)\right)a'\left(0\right)$$
$$+ \left.\sum_{A=1}^{N}\sum_{j=1}^{k}\sum_{m=0}^{j-1}\left(-1\right)^m D_{x,m}\frac{\partial L}{\partial y_j^A}\left(j^{2k-1}s\left(x\right)\right)\cdot\frac{d^{j-m-1}\zeta^A}{dx^{j-m-1}}\right|_a^b$$

and for s a solution of the Euler-Lagrange equations

$$\sum_{j=0}^{k}(-1)^j D_{x.j}\frac{\partial L}{\partial y_j^A}\left(j^{2k}s(x)\right)=0 \text{ for } A=1,2,..N \tag{4}$$

we have

$$\frac{d}{d\varepsilon}|_{\varepsilon=0}\int_{a(e)}^{b(\varepsilon)}L\left(j^k s^{\varepsilon}(x)\right)dx=\theta_{Lag}\left(j^{2k-1}s(b)\right).V_b-\theta_{Lag}\left(j^{2k-1}s(a)\right).V_a \tag{5}$$

where $V_a=\frac{d}{d\varepsilon}|_{\varepsilon=0}a(\varepsilon)\frac{\partial}{\partial x}+\zeta^A|_{x=a(0)}\frac{\partial}{\partial y^A}+\sum_{j=1}^{2k-1}\frac{d^j\zeta^A(x)}{dx^j}|_{x=a(0)}\frac{\partial}{\partial y_j^A}$ is a vector tangent to $J^{2k-1}Y$ at $j^{2k-1}s(a(0))$. V_b is defined analogously, tangent to $J^{2k-1}Y$ at $j^{2k-1}s(b(0))$.

We will prove that a trajectory of the Euler-Lagrange system for a nondegenerate lagrangian is defined by

$$\left(\tilde q(0),\tilde q'(0),...\tilde q^{(k-1)}(0)\right)\in T^{k-1}Q$$
$$\left(\tilde q(h),\tilde q'(h),..\tilde q^{(k-1)}(h)\right)\in T^{k-1}Q$$

The lagrangian is called nondegenerate if the system (4) can be solved for the derivatives of higher order, that is the $Nk\times Nk$ matrix $\left(\frac{\partial^2 L}{\partial y_i^A\partial y_j^B}\right)$ is nonsingular. More precisely we have

Proposition 2. *Let $\tilde q(t)$ a solution of the Euler-Lagrange equations for the nondegenerate lagrangeian $L\left(q,q',..q^{(k)}\right)dt$. Then there exists $h_0>0$ and the neighborhoods V_0 and V_1 of $\left(q(0),q'(0),...q^{(k-1)}(0)\right)$ respectively $(q(h_0),q'(h_0),...$ $..q^{(k-1)}(h_0))$ and a neighborhood V_h of h_0 such that for any $\bar q_0=\left(q_0,v_0^1,v_0^2,..v_0^{k-1}\right)$ $\in V_0$, $\bar q_1=\left(q_1,v_1^1,v_1^2,..v_1^{k-1}\right)\in V_1$ and $h\in V_h$ there exists an unique solution $q_{(\bar q_0,\bar q_1)}(t)$ of the Euler-Lagrange equations such that*

$$q_{(\bar q_0,\bar q_1)}(0)=q_0,\ q'_{(\bar q_0,\bar q_1)}(0)=v_0^1...q_{(\bar q_0,\bar q_1)}^{(k-1)}(0)=v_0^{k-1}$$

$$q_{(\bar q_0,\bar q_1)}(h)=q_1,\ q'_{(\bar q_0,\bar q_1)}(h)=v_1^1...q_{(\bar q_0,\bar q_1)}^{(k-1)}(h)=v_1^{k-1}$$

Proof: We denote $q_{(\bar q_0,\bar q_1)}(t)$ shortly by $\tilde q(t)$. We have the Taylor expantion

$$\tilde q(t)=\tilde q(0)+\frac{\tilde q'(0)}{1!}t+\frac{\tilde q''(0)}{2!}t^2+..\frac{\tilde q^{(2k-1)}(0)}{(2k-1)!}t^{2k-1}+$$

$$+t^{2k}R\left(\tilde q(0),\tilde q'(0),..\tilde q^{(2k-1)}(0),t\right)$$

It is enough to prove that

$$\Delta = \frac{D\left(\tilde{q}(0), \tilde{q}'(0), ..\tilde{q}^{(k-1)}(0), \tilde{q}(h), \tilde{q}'(h)..\tilde{q}^{(k-1)}(h)\right)}{D\left(\tilde{q}(0), \tilde{q}'(0), ..\tilde{q}^{(k-1)}(0), \tilde{q}^{(k)}(0), ..\tilde{q}^{(2k-1)}(0)\right)} \neq 0$$

at

$$\left(\tilde{q}(0), \tilde{q}'(0), ..\tilde{q}^{(k-1)}(0), \tilde{q}^{(k)}(0), ..\tilde{q}^{(2k-1)}(0)\right)$$

for enough small h.

We have

$$\Delta = \det\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

where A, B, C, D are $kN \times kN$ matrices, $A = id_{R^{kn}}$, $B = 0$.

$$D = \begin{pmatrix} \left(\frac{h^k}{k!} + h^{2k}O(1)\right) id & \left(\frac{h^{k+1}}{(k+1)!} + h^{2k}O(1)\right) id & \dots & \left(\frac{h^{2k-1}}{(2k-1)!} + h^{2k}O(1)\right) id \\ \left(\frac{h^{k-1}}{(k-1)!} + h^{2k-1}O(1)\right) id & \left(\frac{h^k}{k!} + h^{2k-1}O(1)\right) id & \dots & \left(\frac{h^{2k-2}}{(2k-2)!} + h^{2k-1}O(1)\right) id \\ \dots & \dots & \dots & \dots \\ \left(\frac{h}{1!} + h^{k+1}O(1)\right) id & \left(\frac{h^2}{2!} + h^{k+1}O(1)\right) id & & \left(\frac{h^k}{k!} + h^{k+1}O(1)\right) id \end{pmatrix}$$

Here id is the $N \times N$ identity matrix. It follows $D = E \otimes id$ and

$$\det(E) = h^{1+2+..+k} \det\begin{pmatrix} \frac{1}{k!} + h^kO(1) & \frac{h}{(k+1)!} + h^kO(1) & .. & \frac{h^{k-1}}{(2k-1)!} + h^kO(1) \\ \frac{1}{(k-1)!} + h^kO(1) & \frac{h}{k!} + h^kO(1) & \dots & \frac{h^{k-1}}{(2k-2)!} + h^kO(1) \\ \dots & \dots & \dots & \\ \frac{1}{1!} + h^kO(1) & \frac{h}{2!} + h^kO(1) & \dots & \frac{h^{k-1}}{k!} + h^kO(1) \end{pmatrix}$$

whence

$$\det(E) = h^{k^2}\left(\det\begin{pmatrix} \frac{1}{k!} & \frac{1}{(k+1)!} & .. & \frac{1}{(2k-1)!} \\ \frac{1}{(k-1)!} & \frac{1}{k!} & \dots & \frac{1}{(2k-2)!} \\ \dots & \dots & \dots & \\ \frac{1}{1!} & \frac{1}{2!} & \dots & \frac{1}{k!} \end{pmatrix} + hO(1)\right)$$

To see that the last determinant is non zero consider the polynomial $p(x)$ of degree 2k-1 having 0 as root of order k and with prescribed values for $p(1)$, $p'(1)$,..$p^{(k-1)}(1)$. Such a polynomial exists and is unique [18]. It can be written $p(x) = a_k \frac{x^k}{k!} + a_{k+1} \frac{x^{k+1}}{(k+1)!} + ... + a_{2k-1} \frac{x^{2k-1}}{(2k-1)!}$. Assigning values for $p(1)$, $p'(1)$,..$p^{(k-1)}(1)$ we get a linear system for a_k, $..a_{2k-1}$ with the matrix

$$F = \begin{pmatrix} \frac{1}{k!} & \frac{1}{(k+1)!} & .. & \frac{1}{(2k-1)!} \\ \frac{1}{(k-1)!} & \frac{1}{k!} & \dots & \frac{1}{(2k-2)!} \\ \dots & \dots & \dots & \\ \frac{1}{1!} & \frac{1}{2!} & \dots & \frac{1}{k!} \end{pmatrix}$$

whence $\det(F) \neq 0$ and it follows $\det(E) \neq 0$ for enough small h and $\det(\Delta) = \det(D) = \det(E \otimes id) \neq 0$.

□

This theorem shows that the exact trajectory of the Euler-Lagrange equations is completely determined by two points and the derivatves up to orders k-1 at these points.

2 Conservative numerical schemes

For discretization of the Euler-Lagrange equations, will take $T^{k-1}Q$ as space of points for discrete trajectory. If locally $Q = R^N$ then $T^{k-1}Q = R^{kN}$ and a point of $T^{k-1}Q$ is $\bar{q} = \left(q, v^1, v^2, .., v^{k-1}\right) \in R^{kN}$ where $q \in Q$ and v^1, v^2, ..,v^{k-1} are the derivatives of orders 1,2,..k-1of a trajectory passing through q. Given two points $\bar{q}_0 = \left(q_0, v_0^1, ..v_0^{k-1}\right) \in T^{k-1}Q$ and $\bar{q}_1 = \left(q_1, v_1^1, ..v_1^{k-1}\right) \in T^{k-1}Q$ enough close then according to (2) the trajectory is uniquely defined. We define the discrete action by

$$S_d\left(\bar{q}_0, \bar{q}_1, h\right) = I_{a,h}\left(L\left(q_{0,1}\left(t\right), q'_{0,1}\left(t\right), ..q_{0,1}^{(k-1)}\left(t\right)\right)\right)$$

where $I_{a,h}$ is a formula of approximate computation for $\int_0^h L\left(q_{0,1}\left(t\right), q'_{0,1}\left(t\right), ..\right.$ $...q_{0,1}^{(k-1)}\left(t\right))dt$, and $q_{0,1}\left(t\right)$ is the polynomial of degree 2k-1 such that $q_{0,1}0) = q_0$, $q_{0,1}^{(i)}\left(0\right) = v_0^i$, i=1..k-1 and, $q_{0,1}\left(h\right) = q_1$, $q_{0,1}^{(i)}\left(h\right) = v_1^i$, i=1..k-1.

We call discrete trajectory a sequence of points $\bar{q}_{dis} = \left(\bar{q}_0, \bar{q}_1, ..\bar{q}_n\right)$, $\bar{q}_i \in T^{k-1}Q$. For every discrete trajectory we define its discrete action by

$$\mathbf{S}_d\left(\bar{q}_{dis}\right) = S_d\left(\bar{q}_0, \bar{q}_1, h\right) + S_d\left(\bar{q}_1, \bar{q}_2, h\right) + ..S_d\left(\bar{q}_{n-1}, \bar{q}_n, h\right)$$

To minimize the action for variations of points $\bar{q}_1$,..$\bar{q}_{n-1}$, (endpoints $\bar{q}_0$ şi $\bar{q}_n$ are fixed) it needs

$$\frac{\partial \mathbf{S}_d}{\partial \bar{q}_1} = 0 \quad \frac{\partial \mathbf{S}_d}{\partial \bar{q}_2} = 0 \quad ... \quad \frac{\partial \mathbf{S}_d}{\partial \bar{q}_{n-1}} = 0 \tag{6}$$

If for threee points $\bar{q}_0$, $\bar{q}_1$, $\bar{q}_2$ the equations (6) are

$$D_2 S_d\left(\bar{q}_0, \bar{q}_1, h\right) + D_1 S_d\left(\bar{q}_1, \bar{q}_2, h\right) = 0 \tag{7}$$

or

$$\frac{\partial}{\partial \bar{q}_1}\left(S_d\left(\bar{q}_0, \bar{q}_1, h\right) + S_d\left(\bar{q}_1, \bar{q}_2, h\right)\right) = 0 \tag{8}$$

where D_1 is the derivative with respect to first argument and D_2 is the derivative with respect to the second argument. These equations are called discrete Euler-Lagrange equations. Solving (8) by respect to $\bar{q}_2$ (if possible) then we get an application $F_h : D \subset T^{k-1}Q \times T^{k-1}Q \to T^{k-1}Q \times T^{k-1}Q$ by the formula

$$F_h\left(\bar{q}_0, \bar{q}_1\right) = \left(\bar{q}_1, \bar{q}_2\right)$$

D is the open set of points $(\bar{q}_0, \bar{q}_1)$ such that exists an continuous trajectory $\tilde{q}(t)$ of the Euler-Lagrange equations as in proposition (2). By iteration we get succesively $(\bar{q}_1, \bar{q}_2) = F_h(\bar{q}_0, \bar{q}_1)$,..,$(\bar{q}_{n-1}, \bar{q}_n) = F_h^n(\bar{q}_0, \bar{q}_1)$. The discrete trajectory $(\bar{q}_0, \bar{q}_1, ..\bar{q}_n)$ fullfils the relations (6).

We have

$$\begin{aligned} d\left(S_d\left(\bar{q}_0, \bar{q}_1, h\right) + F_h^* S_d\left(\bar{q}_0, \bar{q}_1, h\right)\right) &= dS_d\left(\bar{q}_0, \bar{q}_1, h\right) + dS_d\left(\bar{q}_1, \bar{q}_2, h\right) \\ &= D_1 S_d\left(\bar{q}_0, \bar{q}_1, h\right) d\bar{q}_0 + D_2 S_d\left(\bar{q}_1, \bar{q}_2, h\right) d\bar{q}_2 \end{aligned} \tag{9}$$

because of (7).

We define as in [10]

$$\begin{aligned} \Theta^+_{L_d}\left(\bar{q}_0, \bar{q}_1, h\right) &= D_2 S_d\left(\bar{q}_0, \bar{q}_1, h\right) d\bar{q}_1 \\ \Theta^-_{L_d}\left(\bar{q}_0, \bar{q}_1, h\right) &= -D_1 S_d\left(\bar{q}_0, \bar{q}_1, h\right) d\bar{q}_0 \end{aligned}$$

It follows

$$dS_d = \Theta^+_{L_d} - \Theta^-_{L_d} \tag{10}$$

We define the Ω_{L_d} form by

$$\Omega_{L_d} = d\Theta^+_{L_d} = d\Theta^-_{L_d}$$

The equation (9) may be written

$$d\left(S_d\left(\bar{q}_0, \bar{q}_1, h\right) + F_h^* S_d\left(\bar{q}_0, \bar{q}_1, h\right)\right) = \left(F_h^* \Theta^+_{L_d}\right)\left(\bar{q}_0, \bar{q}_1, h\right) - \Theta^-_{L_d}\left(\bar{q}_0, \bar{q}_1, h\right)$$

The exterior derivative of this formula gives

Proposition 3. *Under the above conditions the two form Ω_{L_d} is invariated by F_h, that is*

$$F_h^* \Omega_{L_d} = \Omega_{L_d}$$

□

Using local coordinates, the Ω_{L_d} is expressed by

$$\Omega_{L_d} = \frac{\partial^2 S_d\left(\bar{q}_0, \bar{q}_1, h\right)}{\partial \bar{q}_0 \partial \bar{q}_1} d\bar{q}_0 \wedge d\bar{q}_1 \tag{11}$$

or in more detail

$$\Omega_{L_d} = \frac{\partial^2 S_d\left(\bar{q}_0, \bar{q}_1, h\right)}{\partial q_0^i \partial q_1^j} dq_0^i \wedge dq_1^j + \frac{\partial^2 S_d\left(\bar{q}_0, \bar{q}_1, h\right)}{\partial \left(v_0^r\right)^i \partial \left(v_1^s\right)^j} d\left(v_0^r\right)^i \wedge d\left(v_1^s\right)^j$$
$$+ \frac{\partial^2 S_d\left(\bar{q}_0, \bar{q}_1, h\right)}{\partial q_0^i \partial \left(v_1^s\right)^j} dq_0^i \wedge d\left(v_1^s\right)^j + \frac{\partial^2 S_d\left(\bar{q}_0, \bar{q}_1, h\right)}{\partial \left(v_0^r\right)^i \partial q_1^j} d\left(v_0^r\right)^i \wedge q_1^j \quad (12)$$

The indexes i, j run between 1 and N and the indexes r, s run between 1 and k-1. Remember that $q_0 = \left(q_0^1, q_0^2, ...q_0^N\right) \in R^N$ and $v_0^s = \left(\left(v_0^s\right)^1, \left(v_0^s\right)^2, ... \left(v_0^s\right)^N\right) \in R^N$ in a local representation $\bar{q}_0 = \left(q_0, v_0^1, ..v_0^{k-1}\right)$ for a point in $T^{k-1}Q$.

The accuracy of approximation of the exact trajectory of the Euler-Lagrange equations by the discrete trajectory is measured using a special discrete action (see [10]). Let $\tilde{q}\left(t\right)$ the unique solution of the Euler-Lagrange equations determined by $\bar{q}_0$ and $\bar{q}_1$ as in the proposition (2). Then let

$$S_d^E\left(\bar{q}_0, \bar{q}_1, h\right) = \int_0^h L\left(\tilde{q}\left(t\right), \tilde{q}'\left(t\right), \tilde{q}''\left(t\right), ..\tilde{q}^{(k)}\left(t\right)\right) dt \quad (13)$$

We have the following result:

Proposition 4. *If the discrete action is given by* (13) *and the discrete Euler-Lagrange equations* (8) *are solvable in* $\bar{q}_2$*, then the points of the discrete trajectory generated by* $\left(\bar{q}_0, \bar{q}_1\right)$ *belong to the exact trajectory* $\tilde{q}\left(t\right)$ *of the Euler-Lagrange equations for which* $\tilde{q}\left(0\right) = \bar{q}_0$*,* $\tilde{q}\left(h\right) = \bar{q}_1$.

Proof: We shall prove that on the exact trajectory $\tilde{q}\left(t\right)$ the discrete Euler-Lagrange equations are satisfied at the points $\bar{q}_i = \tilde{q}\left(ih\right)$. The proof is performed for i=1. For other points the proof is analogous. Let $\tilde{q}_\varepsilon$ a variation of $\tilde{q}$ with $\tilde{q}\left(0\right)$ and $\tilde{q}\left(2h\right)$ fixed. From (5) it follows

$$\frac{\partial}{\partial \varepsilon}|_{\varepsilon=0} S_d^E\left(\tilde{q}\left(0\right), \tilde{q}_\varepsilon, h\right) = \theta_{Lag}\left(j^{2k-1}\tilde{q}\left(t\right)\right)|_{t=h}\left(\left.\frac{\partial}{\partial \varepsilon}\right|_{\varepsilon=0} \bar{q}_{1\varepsilon}\right) \quad (14)$$

The same formula for other two points gives

$$\left.\frac{\partial}{\partial \varepsilon}\right|_{\varepsilon=0} S_d^E\left(\tilde{q}_\varepsilon, \tilde{q}\left(2h\right), h\right) = -\theta_{Lag}\left(j^{2k-1}\tilde{q}\left(t\right)\right)|_{t=h}\left(\left.\frac{\partial}{\partial \varepsilon}\right|_{\varepsilon=0} \tilde{q}_\varepsilon\right) \quad (15)$$

From $(14 - 15)$ it follows

$$\frac{\partial}{\partial \bar{q}_1}\left(S_d^E\left(\bar{q}_0, \bar{q}_1, h\right) + S_d^E\left(\bar{q}_1, \bar{q}_2, h\right)\right) = 0$$

that is the discrete Euler-Lagrange equations hold.

□

This proposition implies as in [10] that in case $\left\|\frac{\partial S_d(\bar{q}_1,\bar{q}_2,h)}{\partial \bar{q}_2}\right\| > Ah$ and $\left\|\frac{\partial S_d^E(\bar{q}_1,\bar{q}_2,h)}{\partial \bar{q}_2}\right\| > Ah$ for a positive constant A and

$$\left|S_d^E\left(\bar{q}_0,\bar{q}_1,h\right) - S_d\left(\bar{q}_0,\bar{q}_1,h\right)\right| \leq Ch^{r+2}$$

then

$$\left|F_d^E\left(\bar{q}_0,\bar{q}_1\right) - F_h\left(\bar{q}_0,\bar{q}_1\right)\right| \leq C_1 h^{r+1}.$$

For long times that means$\left|\left(F_d^E\right)^n\left(\bar{q}_0,\bar{q}_1\right) - \left(F_h\right)^n\left(\bar{q}_0,\bar{q}_1\right)\right| \leq C_2 h^r$, $n \approx \frac{1}{h}$ and the method is of order r. Here F_h^E is the map associated to the special action S_d^E, F_h is the map associated to S_d and $\left(\bar{q}_0,\bar{q}_1\right) \in D$. For long times that means

$$\left|\left(F_d^E\right)^n\left(\bar{q}_0,\bar{q}_1\right) - \left(F_h\right)^n\left(\bar{q}_0,\bar{q}_1\right)\right| \leq C_2 h^r, n \approx \frac{1}{h}$$

and the method is of order r. This means that the solutions of the discrete Euler-Lagrange equations are close to that of the exact solution if the discrete action is enough close to the special action.

For practical applications we need interpolations on $[0,h]$ with prescribed values at 0 and h. The third order polynomial with prescribed values $p(0) = q_0$, $p'(0) = v_0$, $p(h) = q_1$, $p'(h) = v_1$ is

$$p(t) = q_0 P_0(t,h) + v_0 R_0(t,h) + q_1 P_1(t,h) + v_1 R_1(t,h) \tag{16}$$

where

$$\begin{aligned} P_0(t,h) &= \frac{(2t+1)(t-h)^2}{h^2} \\ R_0(t,h) &= \frac{t(t-h)^2}{h^2} \\ P_1(t,h) &= \frac{t^2(2(h-t)+1)}{h^2} \\ R_1(t,h) &= \frac{t^2(t-h)}{h^2} \end{aligned}$$

The integrals $\int_0^h P_i(t,h)\,P_j(t,h)\,dt$, $\int_0^h P_i(t,h)\,R_j(t,h)\,dt$ etc. are in the following table

$$\begin{bmatrix} & P_0 & R_0 & P_1 & R_1 \\ P_0 & \frac{13h}{35} & \frac{11h^2}{210} & \frac{9h}{270} & -\frac{13h^2}{210} \\ R_0 & \frac{11h^2}{210} & \frac{h^3}{105} & \frac{13h^2}{420} & -\frac{h^3}{140} \\ P_1 & \frac{9h}{70} & \frac{13h^2}{420} & \frac{13h}{35} & -\frac{11h^2}{210} \\ R_1 & -\frac{13h^2}{420} & -\frac{h^3}{140} & -\frac{11h^2}{210} & \frac{h^3}{105} \end{bmatrix}$$

The integrals $\int_0^h P_i'(t,h)\,P_j'(t,h)\,dt$, $\int_0^h P_i'(t,h)\,R_j'(t,h)\,dt$, etc are in the following

$$\begin{bmatrix} & P_0' & R_0' & P_1' & R_1' \\ P_0' & \frac{6}{5h} & \frac{1}{10} & -\frac{6}{5h} & \frac{1}{10} \\ R_0' & \frac{1}{10} & \frac{2h}{15} & -\frac{1}{10} & -\frac{h}{30} \\ P_1' & -\frac{6}{5h} & -\frac{1}{10} & \frac{6}{5h} & -\frac{1}{10} \\ R_1' & \frac{1}{10} & -\frac{h}{30} & -\frac{1}{10} & \frac{2h}{15} \end{bmatrix}$$

The integrals $\int_0^h P_i''(t,h)\,P_j''(t,h)\,dt$, $\int_0^h P_i''(t,h)\,R_j''(t,h)\,dt$, etc are in the following table

$$\begin{bmatrix} & P_0'' & R_0'' & P_1'' & R_1'' \\ P_0'' & \frac{12}{h^3} & \frac{6}{h^2} & -\frac{12}{h^3} & \frac{6}{h^2} \\ R_0'' & \frac{6}{h^2} & \frac{4}{h} & -\frac{6}{h^2} & \frac{2}{h} \\ P_1'' & -\frac{12}{h^3} & -\frac{6}{h^2} & \frac{12}{h^3} & -\frac{6}{h^2} \\ R_1'' & \frac{6}{h^2} & \frac{2}{h} & -\frac{6}{h^2} & \frac{4}{h} \end{bmatrix}$$

In the sequel we give an example of such a conservatve scheme.

Example 5. *Let*

$$\mathcal{L} = \frac{1}{2} q''^t A q'' - V(q) \tag{17}$$

with A symmetric nonsingular matrix. We define the discrete action using the polynomial (16) *(denoted here by $q_{0,1}(t)$) by*

$$S_d(\bar{q}_0, \bar{q}_1, h) = \int_0^h \left(\frac{1}{2} q''^t_{0,1}(t)\, A q''_{0,1}(t) - V(q_{0,1}(t)) \right) dt$$

Using the preceeding tables it follows

$$\int_0^h \frac{1}{2} q''^t_{0,1}(t)\, A q''_{0,1}(t)\, dt =$$

$$= \frac{1}{h^3} \begin{pmatrix} h^2 v_1 A v_1 + h^2 v_0 A v_1 - 3h q_1 A v_1 + 3h q_0 A v_1 + h^2 v_0 A v_0 \\ -3h q_1 A v_0 + 3h q_0 A v_0 + 3 q_1 A q_1 + 3 q_0 A q_0 - 6 q_0 A q_1 \end{pmatrix}$$

The integral $\int_0^h (-V(q_{0,1}(t)))\,dt$ is approximated by $-hV(q_0)$. We get

$$S_d(\bar{q}_0, \bar{q}_1, h)$$

$$= \frac{1}{h^3} \begin{pmatrix} h^2 v_1 A v_1 + h^2 v_0 A v_1 - 3h q_1 A v_1 + 3h q_0 A v_1 + h^2 v_0 A v_0 \\ -3h q_1 A v_0 + 3h q_0 A v_0 + 3 q_1 A q_1 + 3 q_0 A q_0 - 6 q_0 A q_1 \end{pmatrix} - hV(q_0) \tag{18}$$

Analogously

$$S_d(\bar{q}_1, \bar{q}_2, h) =$$

$$= \frac{1}{h^3} \begin{pmatrix} h^2 v_2 A v_2 + h^2 v_1 A v2 - 3h q_2 A v_2 + 3h q_1 A v_2 + h^2 v_1 A v_1 \\ -3h q_2 A v_1 + 3h q_1 A v_1 + 3 q_2 A q_2 + 3 q_1 A q_1 - 6 q_1 A q_2 \end{pmatrix} - hV(q_1)$$

The discrete Euler-Lagrange equations (8) *are*

$$\frac{6}{h^3}A\left(-2q_0 - hv_0 + 4q_1 - 2q_2 + hv_2\right) - h\nabla V\left(q_1\right) = 0$$
$$\frac{2}{h^2}\left(3q_0 + hv_0 + 4hv_1 - 3q_2 + hv_2\right) = 0$$

whence

$$q_2 = 5q_0 + 2hv_0 + 4hv_1 - 4q_1 + \frac{h^4}{6}A^{-1}\nabla V\left(q_1\right) \tag{19}$$
$$v_2 = \frac{1}{2h}\left(24q_0 - 24q_1 + 10hv_0 + 16hv_1 + h^4A^{-1}\nabla V\left(q_1\right)\right) \tag{20}$$

The Ω_d *form according to* (11) *or* (12) *is*

$$\Omega_d = \frac{1}{h^3}\left(h^2A_{i,j}dv_0^i \wedge dv_1^j + 3hA_{i,j}dq_0^i \wedge dv_1^j - 3hA_{i,j}dv_0^i \wedge dq_1^j - 6A_{i,j}dq_0^i \wedge dq_1^j\right)$$

The Euler-Lagrange equations are not allways solvable with respect to $\bar{q}_2$. If we should use in the preceeding example

$$S_d\left(\bar{q}_0, \bar{q}_1, h\right) = \int_0^h L\left(\tilde{q}\left(t\right), \tilde{q}'\left(t\right), \tilde{q}''\left(t\right)\right)dt \approx S_d\left(\bar{q}_0, \bar{q}_1, h\right) = hL\left(q_0, v_0, \frac{v_1 - v_0}{h}\right)$$

then the discrete Euler-Lagrange equations can't be solved for $\bar{q}_2 = (q_2, v_2)$ and the same things happens if $S_d\left(\bar{q}_0, \bar{q}_1, h\right) = hL\left(q_0, \frac{q_1-q_0}{h}, \frac{v_1-v_0}{h}\right)$.

To find the order of convergency of F_h given by $(19 - 20)$ we compare $\bar{q}_2 = (q_2, v_2)$ with $\left(\tilde{q}\left(2h\right), \tilde{q}'\left(2h\right)\right)$ from the exact solution of the Euler-Lagrange equation passing trough $\bar{q}_0$ and $\bar{q}_1$. For the lagrangeian(17) the equations are

$$q^{(4)} = A^{-1}\nabla V\left(q\right) \tag{21}$$

The exact solution is

$$\tilde{q}\left(t\right) = \tilde{q}\left(0\right) + \tilde{q}'\left(0\right)t + \frac{\tilde{q}''\left(0\right)}{2!}t^2 + \frac{\tilde{q}'''\left(0\right)}{3!}t^3 + \frac{\tilde{q}^{(4)}\left(0\right)}{4!}t^4 + t^5O\left(1\right)$$

The conditions

$$\tilde{q}\left(0\right) = q_0,\ \tilde{q}'\left(0\right) = v_0,\ \tilde{q}\left(h\right) = q_1,\ \ \tilde{q}'\left(h\right) = v_1$$

and (21) imply

$$\tilde{q}\left(t\right) = q_0 + v_0t + \frac{\tilde{q}''\left(0\right)}{2!}t^2 + \frac{\tilde{q}'''\left(0\right)}{3!}t^3 + \frac{A^{-1}\nabla V\left(q_0\right)}{4!}t^4 + t^5O\left(1\right) \tag{22}$$

where

$$\tilde{q}''(0) = \frac{-24hv_1 - 48hv_0 + 72q_1 - 72q_0 + h^4 A^{-1}\nabla V(q_0) + h^5 O(1)}{12h^2}$$
$$\tilde{q}'''(0) = \frac{-24q_1 + 24q_0 + 12hv_0 + 12hv_1 - h^4 A^{-1}\nabla V(q_0) + h^5 O(1)}{2h^3}$$

Finally we get from (22)

$$\tilde{q}(2h) = 5q_0 + 2hv_0 + 4hv_1 - 4q_1 + \frac{h^4}{6} A^{-1}\nabla V(q_0) + h^5 O(1)$$
$$\tilde{q}'(2h) = \frac{1}{2h}\left(24q_0 - 24q_1 + 10hv_0 + 16hv_1 + h^4 A^{-1}\nabla V(q_0)\right) + h^4 O(1)$$

whence

$$\tilde{q}(2h) - q_2 = \frac{h^4}{6} A^{-1}(\nabla V(q_0) - \nabla V(q_1)) + h^5 O(1)$$
$$= h^5 O(1)$$

and

$$\tilde{q}'(2h) - v_2 = \frac{h^3}{2}(\nabla V(q_0) - \nabla V(q_1)) + h^4 O(1)$$
$$= h^4 O(1)$$

These formulas show that the scheme $(19 - 20)$ is of order 3.

3 Numerical experiments

Let the lagrangianl $\mathcal{L} = \frac{a}{2}q''^2 + \frac{b}{2}q'^2$. The next computations were carried out using Mathcad Professional and the results are taken directly from it. The approximate solution determined by $\bar{q}_0 = (q_0,\ v_0)$, $\bar{q}_1 = (q_1,\ v_1)$ according to (16) is

$$q(t, q0, v0, q1, v1, h) := q0 \cdot p0(t,h) + v0 \cdot r0(t,h) + q1 \cdot p1(t,h) + v1 \cdot r1(t,h)$$

The discret action $Sd(\bar{q}_0, \bar{q}_1, h)$ is

$$\int_0^h \left(\frac{d^2}{dt^2} q(t, q0, v0, q1, v1, h)\right)^2 \cdot \frac{a}{2}\, dt + \int_0^h \left(\frac{d^1}{dt^1} q(t, q0, v0, q1, v1, h)\right)^2 \cdot \frac{b}{2}\, dt$$

which expands to

$$\frac{1}{30}\cdot\frac{\begin{pmatrix}2\cdot v1^2\cdot b\cdot h^4+60\cdot v1^2\cdot a\cdot h^2-v1\cdot b\cdot v0\cdot h^4-3\cdot v1\cdot h^3\cdot b\cdot q1\ \ldots\\ +3\cdot v1\cdot h^3\cdot b\cdot q0+60\cdot v1\cdot a\cdot v0\cdot h^2-180\cdot v1\cdot h\cdot a\cdot q1\ \ldots\\ +180\cdot v1\cdot h\cdot a\cdot q0+2\cdot v0^2\cdot b\cdot h^4-3\cdot h^3\cdot b\cdot v0\cdot q1+3\cdot h^3\cdot b\cdot q0\cdot v0\ \ldots\\ +60\cdot h^2\cdot a\cdot v0^2+18\cdot h^2\cdot b\cdot q0^2+18\cdot h^2\cdot b\cdot q1^2-36\cdot h^2\cdot b\cdot q0\cdot q1-180\cdot h\cdot a\cdot v0\cdot q1\ \ldots\\ +180\cdot h\cdot a\cdot q0\cdot v0+180\cdot a\cdot q1^2+180\cdot a\cdot q0^2-360\cdot a\cdot q0\cdot q1\end{pmatrix}}{h^3}$$

The equation $\frac{\partial Sd(\bar{q}_0,\bar{q}_1,h)}{\partial q_1}+\frac{\partial Sd(\bar{q}_1,\bar{q}_2,h)}{\partial q_1}=0$ becomes

$$\frac{1}{10}\cdot\frac{\begin{pmatrix}-h^3\cdot b\cdot v0+24\cdot h^2\cdot b\cdot q1-12\cdot h^2\cdot b\cdot q0-60\cdot h\cdot a\cdot v0+240\cdot a\cdot q1-120\cdot a\cdot q0\ \ldots\\ +v2\cdot h^3\cdot b+60\cdot v2\cdot h\cdot a-12\cdot h^2\cdot b\cdot q2-120\cdot a\cdot q2\end{pmatrix}}{h^3}=0$$

and the equation $\frac{\partial Sd(\bar{q}_0,\bar{q}_1,h)}{\partial v_1}+\frac{\partial Sd(\bar{q}_1,\bar{q}_2,h)}{\partial v_1}=0$ is

$$\frac{1}{(30\cdot h^2)}\cdot\begin{pmatrix}8\cdot v1\cdot h^3\cdot b+240\cdot v1\cdot h\cdot a-h^3\cdot b\cdot v0+3\cdot h^2\cdot b\cdot q0\ \ldots\\ +60\cdot h\cdot a\cdot v0+180\cdot a\cdot q0-v2\cdot h^3\cdot b+60\cdot v2\cdot h\cdot a-3\cdot h^2\cdot b\cdot q2-180\cdot a\cdot q2\end{pmatrix}=0$$

The solution of these two equations is

$$Q2(q0,v0,q1,v1,h,a,b):=\frac{1}{15}\cdot\frac{\begin{pmatrix}7200\cdot h\cdot a^2\cdot v0-9\cdot h^4\cdot b^2\cdot q0\ \ldots\\ +24\cdot h^4\cdot b^2\cdot q1-2\cdot h^5\cdot b^2\cdot v0-14400\cdot a^2\cdot q1\ \ldots\\ +18000\cdot a^2\cdot q0-1200\cdot h^2\cdot b\cdot a\cdot q1+960\cdot h^2\cdot b\cdot a\cdot q0\ \ldots\\ +14400\cdot v1\cdot h\cdot a^2+8\cdot v1\cdot h^5\cdot b^2+720\cdot v1\cdot h^3\cdot b\cdot a\end{pmatrix}}{(h^4\cdot b^2-16\cdot h^2\cdot b\cdot a+240\cdot a^2)}$$

$$V2(q0,v0,q1,v1,h,a,b):=\frac{1}{5}\cdot\frac{\begin{pmatrix}6000\cdot h\cdot a^2\cdot v0+9600\cdot v1\cdot h\cdot a^2-14400\cdot a^2\cdot q1+14400\cdot a^2\cdot q0\ \ldots\\ +320\cdot h^3\cdot b\cdot a\cdot v0\ \ldots\\ +1680\cdot h^2\cdot b\cdot a\cdot q0-1680\cdot h^2\cdot b\cdot a\cdot q1+1280\cdot v1\cdot h^3\cdot b\cdot a\ \ldots\\ +32\cdot v1\cdot h^5\cdot b^2-3\cdot h^5\cdot b^2\cdot v0\ \ldots\\ +24\cdot h^4\cdot b^2\cdot q0-24\cdot h^4\cdot b^2\cdot q1\end{pmatrix}}{[h\cdot(h^4\cdot b^2-16\cdot h^2\cdot b\cdot a+240\cdot a^2)]} \tag{23}$$

For a=1 and b=-1 the exact solution is

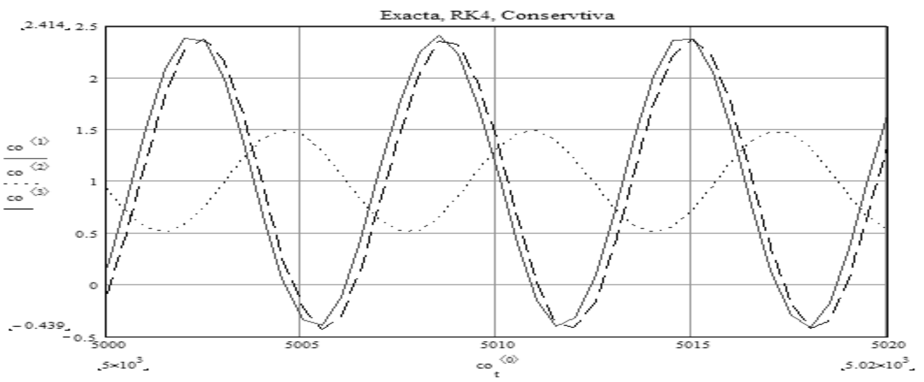
$$C_1+C_2t+C_3\cos t+C_4\sin t$$

A bounded solution is

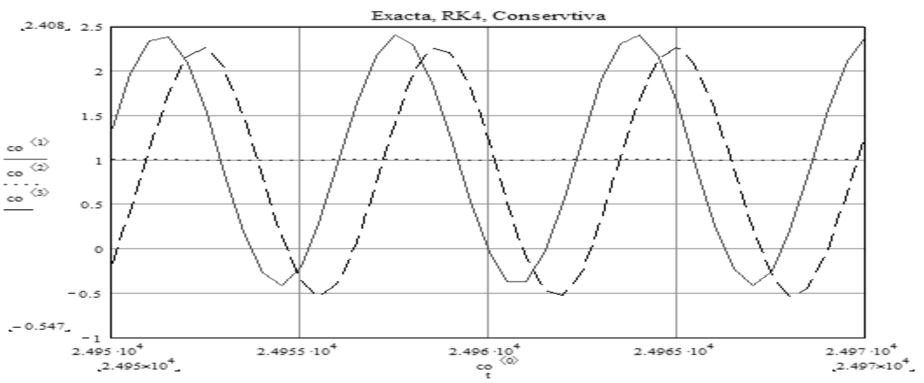
$$1+\cos t+\sin t$$

We shall approximate this solution with the values given by the conservative method (23) and with the values given by the classical Runge-Kutta four step method, with the step h=0,5.

For small values of t, the values obtained with the conservative method and the Runge-Kutta method practically coincide with the exact values. As t grows, the values obtained with the Runge-Kutta method tend to 1. The values obtained with the conservative method are little translated from the exact solution.



The exact and aproximate solution after 10000 steps of numerical integration



The exact and aproximate solution after 50000 steps of numerical integration

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