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 \( \text{Lag} = L(y, y', y'', \ldots y^{(k)}) \, dx \)

Key Words: jet space, Cartan form, lagrangian, conservative numerical scheme.

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1 Preliminaries

Let consider the fibration of \( \pi_{XY} : Y \to X \) 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 \( (y^1, y^2, \ldots y^N) \) are local coordinates on Q, then on \( J^k Y \) we use the coordinates \( (x, y^A, y^A_i)_{A=1..A, i=1..k} \) where for the jet of a section \( s : X \to Y \), \( s(x) = (x, s^1(x), s^2(x), \ldots s^N(x)) \) we have \( y^A = s^A(x) \), \( y^A_i = \frac{\partial}{\partial x^i} s^A(x) \). In the following \( y^A_0 \) is identical to \( y^A \). The correspondence \( x \to j^k s(x) \) is a section of \( J^k Y \) and is denoted by \( j^k s \). By truncation of a k development to a l development \( (l < k) \) we get a projection \( \pi_{J^l Y, J^k Y} : J^k Y \to J^l Y \).

Using local coordinates we define the total derivative \( D_x = \frac{\partial}{\partial x} + y^1 \frac{\partial}{\partial y^1} + y^2 \frac{\partial}{\partial y^2} + \ldots + y^N \frac{\partial}{\partial y^N} + y^A_i \frac{\partial}{\partial y^A_i} + y^A_{i+1} \frac{\partial}{\partial y^A_i} \) as a function from \( J^{k+1} Y \) to the tangent space \( T J^k Y \) and we define also the differential forms \( \theta^A_0 = \theta^A = dy^A - y^A_0 \, dx \), \( \theta^A_j = dy^A_j - y^A_{j+1} \, dx \), for \( j \geq 1 \). For any section \( s \) we have \( j^k s^* (\theta^A_j) = 0 \), and \( \theta^A_j (D_x) = 0 \). By lagrangian on \( J^k Y \) we understand a differential form of degree 1 which
to any jet $\gamma \in J^kY$ takes value in $\pi_{X,J^kY}^* (\Lambda^1X)$. Using local coordinates, a lagrangian is a differential form

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

Any function $f: J^kY \to R$ can be considered as a function denoted abusively also, defined on any $J^nY$ $(n>k)$ by the composition $J^mY \xrightarrow{\pi_{J^kY,J^nY}} J^kY \xrightarrow{f} R$. 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 $f: J^pY \to R$, a function $D_{x,p} f: J^{k+p}Y \to R$, by the formula $D_{x,p} f = D_x D_x ... D_x (f)$. For $p=0$ we define $D_{x,0} = \text{identity}$. For a section $s$ of $Y$ we have

$$\frac{d}{dx} \left( f (x, s^A (x), d s^A (x)/dx, ... , d^k s^A (x)/dx^k) \right)$$

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

We have the following result:

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

$$\theta_{\text{Lag}} = L dx + \sum_{A=1}^{N} \sum_{b=1}^{k} \sum_{m=0}^{j-1} (-1)^m D_{x,m} \frac{\partial L}{\partial y_j^A} \cdot \theta_j^{A,m-1} \tag{2}$$

$$= L dx + \sum_{A=1}^{N} \sum_{b=1}^{k} \sum_{m=0}^{b-1} (-1)^m D_{x,m} \frac{\partial L}{\partial y_{m+b+1}^A} \cdot \theta_b^A \tag{3}$$

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

For a proof see [15]. □

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

$$\frac{d}{dx} |_{x=0} \int_{a (\varepsilon)}^{b (\varepsilon)} L (j^k s^\varepsilon (x)) \, dx = \sum_{A=1}^{N} \sum_{j=0}^{k} \int_a^b (-1)^j D_{x,j} \frac{\partial L}{\partial y_j^A} (j^k s^\varepsilon (x)) \cdot \varepsilon^A (x) \, dx$$

$$+ L (j^k s (b)) b' (0) - L (j^k s (a)) a' (0)$$

$$+ \left[ \sum_{A=1}^{N} \sum_{j=1}^{k} \sum_{m=0}^{j-1} (-1)^m D_{x,m} \frac{\partial L}{\partial y_j^A} (j^{2k-1} s^\varepsilon (x)) \cdot \frac{d^{j-m-1} \varepsilon^A}{dx^{j-m-1}} \right] \bigg|_a^b$$
Proposition 2. More precisely we have
\[ V_t \text{ tangent to } J V \]
where
\[ V \in L \text{ degenerate lagrangeian} \]
and for s a solution of the Euler-Lagrange equations
\[ V \in L \text{ degenerate lagrangeian} \]
\[ \forall \alpha \neq \beta \]
\[ V_\alpha \text{ is defined analogously, tangent to } J^{2k-1}Y \text{ at } J^{2k-1}s(\alpha(0)). \]

We will prove that a trajectory of the Euler-Lagrange system for a nondegenerate lagrangian is defined by
\[ \left( \tilde{q}(0), \tilde{q}'(0), \ldots, \tilde{q}^{(k-1)}(0) \right) \in T^{k-1}Q \]
\[ \left( \tilde{q}(h), \tilde{q}'(h), \ldots, \tilde{q}^{(k-1)}(h) \right) \in T^{k-1}Q \]
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 \( \frac{\partial^2 L}{\partial y^\alpha \partial y^\beta} \) is nonsingular.

More precisely we have

**Proposition 2.** Let \( \tilde{q}(t) \) a solution of the Euler-Lagrange equations for the nondegenerate lagrangian \( L(q, q', \ldots q^{(k)}) \) \( \alpha \neq \beta \). Then there exists \( h_0 \) > 0 and the neighborhoods \( V_0 \) and \( V_1 \) of \( (q(0), q'(0), \ldots q^{(k-1)}(0)) \) respectively \( (q(h_0), q'(h_0), \ldots, q^{(k-1)}(h_0)) \) and a neighborhood \( V_h \) of \( h_0 \) such that for any \( \tilde{q}_0 = (q_0, v_0^1, v_0^2, \ldots v_0^{k-1}) \) \( \in V_0 \), \( q_1 = (q_1, v_1^1, v_1^2, \ldots v_1^{k-1}) \) \( \in V_1 \) and \( h \in V_h \) there exists an unique solution \( q_{(\tilde{q}_0, q_1)}(t) \) of the Euler-Lagrange equations such that

\[
q_{(\tilde{q}_0, q_1)}(0) = q_0, \quad q_{(\tilde{q}_0, q_1)}'(0) = v_0^1, \ldots q_{(\tilde{q}_0, q_1)}^{(k-1)}(0) = v_0^{k-1} \\
q_{(\tilde{q}_0, q_1)}(h) = q_1, \quad q_{(\tilde{q}_0, q_1)}'(h) = v_1^1, \ldots q_{(\tilde{q}_0, q_1)}^{(k-1)}(h) = v_1^{k-1} 
\]

**Proof:** We denote \( q_{(\tilde{q}_0, q_1)}(t) \) shortly by \( \tilde{q}(t) \). We have the Taylor expansion
\[ \tilde{q}(t) = \tilde{q}(0) + \frac{\tilde{q}'(0)}{1!} t + \frac{\tilde{q}''(0)}{2!} t^2 + \ldots + \frac{\tilde{q}^{(2k-1)}(0)}{(2k-1)!} t^{2k-1} + \]
\[ + t^{2k} R \left( \tilde{q}(0), \tilde{q}'(0), \ldots, \tilde{q}^{(2k-1)}(0), t \right) \]
It is enough to prove that
\[
\Delta = \frac{D (\tilde{q} (0), \tilde{q}' (0), \ldots \tilde{q}^{(k-1)} (0), \tilde{q} (h), \tilde{q}' (h), \ldots \tilde{q}^{(k-1)} (h))}{D (\tilde{q} (0), \tilde{q}' (0), \ldots \tilde{q}^{(k-1)} (0), \tilde{q}^{(k)} (0), \ldots \tilde{q}^{(2k-1)} (0))} \neq 0
\]
at
\[
\left(\tilde{q} (0), \tilde{q}' (0), \ldots \tilde{q}^{(k-1)} (0), \tilde{q}^{(k)} (0), \ldots \tilde{q}^{(2k-1)} (0)\right)
\]
for enough small h.

We have
\[
\Delta = \det \left( \begin{array}{cc} A & B \\ C & D \end{array} \right)
\]
where A, B, C, D are \( kN \times kN \) matrices, \( A = \text{id}_{R^{kn}} \), \( B = 0 \).

\[
D = \begin{pmatrix}
\left(\frac{k}{h} + h^k O(1)\right) id & \left(\frac{k^2}{h} + h^k O(1)\right) id & \ldots & \left(\frac{k^2}{h} + h^k O(1)\right) id \\
\left(\frac{k}{h} + h^k O(1)\right) id & \left(\frac{k}{h} + h^k O(1)\right) id & \ldots & \left(\frac{k}{h} + h^k O(1)\right) id \\
\left(\frac{k}{h} + h^k O(1)\right) id & \ldots & \ldots & \left(\frac{k}{h} + h^k O(1)\right) id \\
\left(\frac{k}{h} + h^k O(1)\right) id & \ldots & \ldots & \left(\frac{k}{h} + h^k O(1)\right) id
\end{pmatrix}
\]

Here \( \text{id} \) is the \( N \times N \) identity matrix. It follows \( D = E \otimes \text{id} \) and

\[
\det (E) = h^{k+2} \ldots h \det \left( \begin{array}{cccc}
\frac{1}{h} + h^k O(1) & \frac{k}{h} + h^k O(1) & \ldots & \frac{k^2}{h} + h^k O(1) \\
\frac{k}{h} + h^k O(1) & \frac{k}{h} + h^k O(1) & \ldots & \frac{k}{h} + h^k O(1) \\
\frac{1}{h} + h^k O(1) & \frac{1}{h} + h^k O(1) & \ldots & \frac{k^2}{h} + h^k O(1) \\
\frac{1}{h} & \frac{1}{h} & \ldots & \frac{1}{h}
\end{array} \right)
\]

whence

\[
\det (E) = h^{k^2} \left( \det \left( \begin{array}{cccc}
\frac{1}{h^2} & \frac{1}{(k+1)!} & \ldots & \frac{1}{(2k-1)!} \\
\frac{1}{k!} & \frac{1}{k!} & \ldots & \frac{1}{k!} \\
\ldots & \ldots & \ldots & \ldots \\
\frac{1}{k!} & \frac{1}{k!} & \ldots & \frac{1}{k!}
\end{array} \right) + h O(1) \right)
\]

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 \( p(1) \), \( p'(1), \ldots, p^{(k-1)}(1) \). Such a polynomial exists and is unique [18]. It can be written \( p(x) = a_k \frac{x^k}{k!} + a_{k+1} \frac{x^{k+1}}{(k+1)!} + \ldots + a_{2k-1} \frac{x^{2k-1}}{(2k-1)!} \). Assigning values for \( p(1), p'(1), \ldots, p^{(k-1)}(1) \) we get a linear system for \( a_k, \ldots, a_{2k-1} \) with the matrix

\[
F = \begin{pmatrix}
\frac{1}{k!} & \frac{1}{(k+1)!} & \ldots & \frac{1}{(2k-1)!} \\
\frac{1}{k!} & \frac{1}{k!} & \ldots & \frac{1}{k!} \\
\ldots & \ldots & \ldots & \ldots \\
\frac{1}{k!} & \frac{1}{k!} & \ldots & \frac{1}{k!}
\end{pmatrix}
\]
whence \( \det(F) \neq 0 \) and it follows \( \det(E) \neq 0 \) for enough small \( h \) and \( \det(\Delta) = \det(E \otimes id) \neq 0 \).

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

2 Conserved numerical schemes

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

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

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

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

\[
S_d(\bar{q}_{dis}) = S_d(\bar{q}_0, \bar{q}_1, h) + S_d(\bar{q}_1, \bar{q}_2, h) + \ldots + S_d(\bar{q}_{n-1}, \bar{q}_n, h)
\]

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

\[
\frac{\partial S_d}{\partial \bar{q}_1} = 0 \quad \frac{\partial S_d}{\partial \bar{q}_2} = 0 \quad \ldots \quad \frac{\partial S_d}{\partial \bar{q}_{n-1}} = 0
\]

(6)

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

\[
D_2S_d(\bar{q}_0, \bar{q}_1, h) + D_1S_d(\bar{q}_1, \bar{q}_2, h) = 0
\]

(7)

or

\[
\frac{\partial}{\partial \bar{q}_1} (S_d(\bar{q}_0, \bar{q}_1, h) + S_d(\bar{q}_1, \bar{q}_2, h)) = 0
\]

(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...
\[ F_h (\bar{q}_0, \bar{q}_1) = (\bar{q}_1, \bar{q}_2) \]

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 successively \((\bar{q}_1, \bar{q}_2) = F_h (\bar{q}_0, \bar{q}_1), \ldots (\bar{q}_{n-1}, \bar{q}_n) = F_h^n (\bar{q}_0, \bar{q}_1)\). The discrete trajectory \((\bar{q}_0, \bar{q}_1, \ldots, \bar{q}_n)\) fullfils the relations (6).

We have

\[ d (S_d (\bar{q}_0, \bar{q}_1, h) + F_h^* S_d (\bar{q}_0, \bar{q}_1, h)) = dS_d (\bar{q}_0, \bar{q}_1, h) + dS_d (\bar{q}_1, \bar{q}_2, h) \]

(9)

\[ = D_1 S_d (\bar{q}_0, \bar{q}_1, h) \, d\bar{q}_0 + D_2 S_d (\bar{q}_1, \bar{q}_2, h) \, d\bar{q}_2 \]

because of (7).

We define as in [10]

\[ \Theta^+_{L_d} (\bar{q}_0, \bar{q}_1, h) = D_2 S_d (\bar{q}_0, \bar{q}_1, h) \, d\bar{q}_1 \]

\[ \Theta^-_{L_d} (\bar{q}_0, \bar{q}_1, h) = - D_1 S_d (\bar{q}_0, \bar{q}_1, h) \, d\bar{q}_0 \]

It follows

\[ dS_d = \Theta^+_{L_d} - \Theta^-_{L_d} \]

(10)

We define the \(\Omega_{L_d}\) form by

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

The equation (9) may be written

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

The exterior derivative of this formula gives

**Proposition 3.** Under the above conditions the two form \(\Omega_{L_d}\) is invariated by \(F_h\), that is

\[ F_h^* \Omega_{L_d} = \Omega_{L_d} \]

Using local coordinates, the \(\Omega_{L_d}\) is expressed by

\[ \Omega_{L_d} = \frac{\partial^2 S_d (\bar{q}_0, \bar{q}_1, h)}{\partial \bar{q}_0 \partial \bar{q}_1} d\bar{q}_0 \wedge d\bar{q}_1 \]

(11)

or in more detail
Proposition 4. We have the following result: 

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

The indexes i, j run between 1 and N and the indexes r, s run between 1 and k-1. Remember that \( q_0 = (q_0^1, q_0^2, ..., q_0^N) \in R^N \) and \( v_0 = ((v_0^1)^1, (v_0^2)^2, ..., (v_0^N)^N) \in R^N \). From (14) it follows

\[
S_d^E (\bar{q}_0, h) = \int_0^h L (\bar{q}, \dot{\bar{q}}, \ddot{\bar{q}}, ..., \bar{q}^{(k)} (t)) dt
\] (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 \((\bar{q}_0, \bar{q}_1)\) belong to the exact trajectory \( \bar{q} (t) \) of the Euler-Lagrange equations for which \( \bar{q} (0) = \bar{q}_0, \bar{q} (h) = \bar{q}_1 \).

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

\[
\left. \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} S_d^E (\bar{q}, \varepsilon, h) = \frac{\partial}{\partial \varepsilon} \left. \left( \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} \bar{q}_i \right)
\] (14)

The same formula for other two points gives

\[
\left. \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} S_d^E (\bar{q}, \varepsilon, h) = \left. \frac{\partial}{\partial \varepsilon} \left. \left( \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} \bar{q}_i \right) \right|_{t=h}
\] (15)

From (14 − 15) it follows

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

that is the discrete Euler-Lagrange equations hold. \( \square \)
This proposition implies as in [10] that in case \( \left\| \frac{\partial S_d(q_0, q_1, h)}{\partial q_2} \right\| > Ah \) and
\( \left\| \frac{\partial S_d^E(q_0, q_1, h)}{\partial q_2} \right\| > Ah \) for a positive constant \( A \) and
\[
|S_d^E(q_0, q_1, h) - S_d(q_0, q_1, h)| \leq Ch^{r+2}
\]
then
\[
|F_d^E(q_0, q_1) - F_h(q_0, q_1)| \leq C_1 h^{r+1}.
\]
For long times that means \( |(F_d^E)^n(q_0, q_1) - (F_h)^n(q_0, q_1)| \leq C_2 h^r, n \approx \frac{1}{h} \) and the method is of order \( r \). Here \( F_d^E \) is the map associated to the special action \( S_d \), \( F_h \) is the map associated to \( S_h \) and \( (q_0, q_1) \in D \). For long times that means
\[
|(F_d^E)^n(q_0, q_1) - (F_h)^n(q_0, q_1)| \leq C_2 h^r, n \approx \frac{1}{h}
\]
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
\[
\begin{align*}
P_0(t, h) &= \frac{(2t + 1)(t - h)^2}{h^2} \\
R_0(t, h) &= \frac{t(t - h)^2}{h^2} \\
P_1(t, h) &= \frac{t^2(2(h - t) + 1)}{h^2} \\
R_1(t, h) &= \frac{t^2(t - h)}{h^2}
\end{align*}
\]
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
\[
\begin{bmatrix}
P_0 & P_1 & R_0 & R_1 \\
P_0 & 1.3h^2 & 11h^2 & 2 \frac{9h}{10} & -1.3h^2 & 210h \\
P_0 & 1.3h^2 & 11h^2 & 2 \frac{9h}{10} & -1.3h^2 & 210h \\
P_0 & 1.3h^2 & 11h^2 & 2 \frac{9h}{10} & -1.3h^2 & 210h \\
P_0 & 1.3h^2 & 11h^2 & 2 \frac{9h}{10} & -1.3h^2 & 210h
\end{bmatrix}
\]
The integrals $\int_0^h P_i^o (t, h) P_j^o (t, h) \, dt$, $\int_0^h P_i^p (t, h) R_j^p (t, h) \, dt$, etc are in the following table:

\[
\begin{bmatrix}
P_0^o & P_0^p & R_0^p & R_1^p \\
P_0^p & 0 & 0 & 0 \\
R_0^o & 0 & 0 & 0 \\
R_1^o & 0 & 0 & 0
\end{bmatrix}
\]

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

\[
\begin{bmatrix}
P_0^{op} & P_0^{op} & P_1^{op} & R_1^{op} \\
P_0^{op} & 0 & 0 & 0 \\
R_0^{op} & 0 & 0 & 0 \\
R_1^{op} & 0 & 0 & 0
\end{bmatrix}
\]

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

**Example 5.** Let

\[ L = \frac{1}{2} q^{'''} (t) \cdot \sum q^{'''} (t) - V (q) \]  

(17)

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

\[ S_d (q_0, q_1, h) = \int_0^h \left( \frac{1}{2} q_{1,1}^{'''} (t) A q_{1,1}^{'''} (t) - V (q_{1,1} (t)) \right) \, dt \]

Using the preceding tables it follows

\[
\int_0^h \frac{1}{2} q_{1,1}^{'''} (t) A q_{1,1}^{'''} (t) \, dt =
\]

\[
= \frac{1}{h^3} \left( h^2 v_1 A v_1 + h^2 v_0 A v_1 - 3 h q_1 A v_1 + 3 b q_0 A v_1 + h^2 v_0 A v_0 \right)
\]

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

\[ S_d (q_0, q_1, h) =
\]

\[
= \frac{1}{h^3} \left( h^2 v_1 A v_1 + h^2 v_0 A v_1 - 3 h q_1 A v_1 + 3 b q_0 A v_1 + h^2 v_0 A v_0 \right) - h V (q_0) \]  

(18)

Analogously

\[ S_d (q_1, q_2, h) =
\]

\[
= \frac{1}{h^3} \left( h^2 v_2 A v_2 + h^2 v_1 A v_2 - 3 h q_2 A v_2 + 3 h q_1 A v_2 + h^2 v_1 A v_1 \right) - h V (q_1)
\]
The discrete Euler-Lagrange equations (8) are

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

\[
\frac{2}{h^2} (3q_0 + hv_0 + 4hv_1 - 3q_2 + hv_2) = 0
\]

whence

\[
q_2 = 5q_0 + 2hv_0 + 4hv_1 - 4q_1 + \frac{h^4}{6} A^{-1} \nabla V (q_1)
\]

(19)

\[
v_2 = \frac{1}{2h} (24q_0 - 24q_1 + 10hv_0 + 16hv_1 + h^4 A^{-1} \nabla V (q_1))
\]

(20)

The Euler-Lagrange equations are not always solvable with respect to \( \bar{q}_2 \). If we should use in the preceding example

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

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

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

\[
q^{(4)} = A^{-1} \nabla V (q)
\]

(21)

The exact solution is

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

The conditions

\[
\tilde{q} (0) = q_0, \quad \tilde{q}' (0) = v_0, \quad \tilde{q} (h) = q_1, \quad \tilde{q}' (h) = v_1
\]

and (21) imply

\[
\bar{q} (t) = q_0 + v_0 t + \frac{\tilde{q}'' (0)}{2!} t^2 + \frac{\tilde{q}''' (0)}{3!} t^3 + \frac{A^{-1} \nabla V (q_0)}{4!} t^4 + t^5 O (1)
\]

(22)
where
\[ \ddot{q}'(0) = -\frac{24h v_1 - 48h v_0 + 72q_1 - 72q_0 + h^4 A^{-1} \nabla V(q_0) + h^5 O(1)}{12h^2} \]
\[ \dddot{q}'(0) = -\frac{24q_1 + 24q_0 + 12h v_0 + 12h v_1 - h^4 A^{-1} \nabla V(q_0) + h^5 O(1)}{2h^3} \]

Finally we get from (22)
\[ \ddot{q}(2h) = 5q_0 + 2hv_0 + 4hv_1 - 4q_1 + h^4 A^{-1} \nabla V(q_0) + h^5 O(1) \]
\[ \dddot{q}(2h) = \frac{1}{2h} (24q_0 - 24q_1 + 10h v_0 + 16h v_1 + h^4 A^{-1} \nabla V(q_0)) + h^5 O(1) \]
whence
\[ \ddot{q}(2h) - q_2 = h^4 \left( \frac{A^{-1}}{6} (\nabla V(q_0) - \nabla V(q_1)) \right) + h^5 O(1) \]
\[ \dddot{q}(2h) - v_2 = h^3 \left( \frac{1}{2} (\nabla V(q_0) - \nabla V(q_1)) \right) + h^4 O(1) \]
and
\[ \ddot{q}'(2h) - v_2 = h^3 \left( \frac{1}{2} (\nabla V(q_0) - \nabla V(q_1)) \right) + h^4 O(1) \]

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

3 Numerical experiments

Let the lagrangian \( L = \frac{1}{2} q'^2 + \frac{1}{2} q^2 \). 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

\[ q(t, q_0, v_0, q_1, v_1, h) := q_0 \cdot p_0(t, h) + v_0 \cdot r_0(t, h) + q_1 \cdot p_1(t, h) + v_1 \cdot r_1(t, h) \]

The discret action \( S_d(q_0, q_1, h) \) is

\[ \int_0^h \left( \frac{d^2}{dt^2} q(t, q_0, v_0, q_1, v_1, h) \right)^2 \frac{2}{3} dt - \int_0^h \left( \frac{d}{dt} q(t, q_0, v_0, q_1, v_1, h) \right)^2 \frac{b}{2} dt \]
which expands to

\[
\begin{pmatrix}
2 \cdot v1^2 \cdot b \cdot h^4 + 60 \cdot v1^2 \cdot a \cdot h^2 - v1 \cdot b \cdot v_0 - h^3 - 3 \cdot v1 \cdot h^2 \cdot b \cdot v_1 \\
+ 3 \cdot v1 \cdot h^2 \cdot b \cdot v_0 + 60 \cdot v1 \cdot a \cdot v_0 \cdot h^2 - 180 \cdot v1 \cdot h \cdot a \cdot v_0 \\
+ 150 \cdot v1 \cdot h \cdot a \cdot v_0 + 2 \cdot v_0^2 \cdot b \cdot h^4 - 3 \cdot h^2 \cdot b \cdot v_0 \cdot q_1 + 3 \cdot h^2 \cdot b \cdot v_0 \cdot q_0 \\
+ 60 \cdot h^2 \cdot a \cdot v_0^2 + 15 \cdot h^2 \cdot b \cdot q_0^2 + 15 \cdot h^2 \cdot b \cdot q_1^2 - 36 \cdot h^2 \cdot b \cdot q_0 \cdot q_1 - 180 \cdot h \cdot a \cdot v_0 \cdot q_1
\end{pmatrix}
\]

\[
\frac{1}{30} \begin{pmatrix}
+ 150 \cdot h \cdot a \cdot q_0 \cdot v_0 + 180 \cdot a \cdot q_1^2 + 180 \cdot a \cdot q_0^2 - 360 \cdot a \cdot q_0 \cdot q_1
\end{pmatrix}
\]

The equation \( \frac{\partial Sd(q_0, q_1, h)}{\partial q_1} + \frac{\partial Sd(q_1, q_2, h)}{\partial q_1} = 0 \) becomes

\[
\begin{pmatrix}
-h_1^2 \cdot b \cdot v_0 + 24 \cdot h^2 \cdot b \cdot q_1 - 12 \cdot h^2 \cdot b \cdot q_0 - 60 \cdot h \cdot a \cdot v_0 + 240 \cdot a \cdot q_1 - 120 \cdot a \cdot q_0 \\
-5 \cdot v_1 \cdot h^2 \cdot b + 60 \cdot v_2 \cdot h \cdot a - 12 \cdot h^2 \cdot b \cdot q_2 - 120 \cdot a \cdot q_2
\end{pmatrix}
\]

\[= 0\]

and the equation \( \frac{\partial Sd(q_0, q_1, h)}{\partial v_1} + \frac{\partial Sd(q_1, q_2, h)}{\partial v_1} = 0 \) is

\[
\begin{pmatrix}
600 \cdot h \cdot a \cdot q_0 - 90 \cdot h^4 \cdot b^2 \cdot q_0 \\
+ 320 \cdot h_1^2 \cdot b^2 \cdot q_1 - 1200 \cdot h^2 \cdot b \cdot a \cdot q_1 + 960 \cdot h^2 \cdot b \cdot a \cdot q_0 \\
+ 14400 \cdot v_1 \cdot h \cdot a^2 - 60 \cdot v_1 \cdot h^2 \cdot b^2 + 720 \cdot v_1 \cdot h^2 \cdot b \cdot a
\end{pmatrix}
\]

\[= 0\]

The solution of these two equations is

\[
Q_2(q_0, v_0, q_1, v_1, h, a, b) = \frac{1}{15}
\begin{pmatrix}
7200 \cdot h \cdot a^2 \cdot v_0 - 9 \cdot h^4 \cdot b^2 \cdot q_0 \\
+ 24 \cdot h^3 \cdot b^2 \cdot q_1 - 2 \cdot h^2 \cdot b^2 \cdot v_0 - 14400 \cdot a^2 \cdot q_1 \\
- 18000 \cdot a^2 \cdot q_0 - 1200 \cdot h^2 \cdot b \cdot a \cdot q_1 + 960 \cdot h^2 \cdot b \cdot a \cdot q_0 \\
+ 14400 \cdot v_1 \cdot h \cdot a^2 - 60 \cdot v_1 \cdot h^2 \cdot b^2 + 720 \cdot v_1 \cdot h^2 \cdot b \cdot a
\end{pmatrix}
\]

\[
= \frac{1}{5}
\begin{pmatrix}
6000 \cdot h \cdot a^2 \cdot v_0 + 9600 \cdot v_1 \cdot h \cdot a^2 - 14400 \cdot a^2 \cdot q_1 + 14400 \cdot a^2 \cdot q_0 \\
+ 320 \cdot h_1^2 \cdot b^2 \cdot q_1 \\
+ 18000 \cdot v_1 \cdot h \cdot a^2 - 60 \cdot v_1 \cdot h^2 \cdot b^2 + 720 \cdot v_1 \cdot h^2 \cdot b \cdot a \\
+ 32 \cdot v_1 \cdot h \cdot a^2 - 3 \cdot h_1^2 \cdot b^2 \cdot q_0 \\
+ 24 \cdot h^3 \cdot b^2 \cdot q_0 - 24 \cdot h^3 \cdot b^2 \cdot q_1
\end{pmatrix}
\]

\[= \frac{1}{5}
\begin{pmatrix}
6000 \cdot h \cdot a^2 \cdot v_0 + 9600 \cdot v_1 \cdot h \cdot a^2 - 14400 \cdot a^2 \cdot q_1 + 14400 \cdot a^2 \cdot q_0 \\
+ 320 \cdot h_1^2 \cdot b^2 \cdot q_1 \\
+ 18000 \cdot v_1 \cdot h \cdot a^2 - 60 \cdot v_1 \cdot h^2 \cdot b^2 + 720 \cdot v_1 \cdot h^2 \cdot b \cdot a \\
+ 32 \cdot v_1 \cdot h \cdot a^2 - 3 \cdot h_1^2 \cdot b^2 \cdot q_0 \\
+ 24 \cdot h^3 \cdot b^2 \cdot q_0 - 24 \cdot h^3 \cdot b^2 \cdot q_1
\end{pmatrix}
\]

For \( a=1 \) and \( b=-1 \) the exact solution is

\[C_1 + C_2 t + C_3 \cos t + C_4 \sin t\]

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 approximate solution after 10000 steps of numerical integration

The exact and approximate solution after 50000 steps of numerical integration

References


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