

Integrator for Lagrangian Dynamics

C. Udriște, M. Postolache and I. Țevy

Abstract

In §1 we bring the reader gently along from the theory of discrete single-time Lagrangian dynamics (for details see [3]). §2 develops the theory of discrete multi-time Lagrangian dynamics, emphasizing the possibility of computer modelling via Newton method (for details see [8], [9]).

Mathematics Subject Classification: 49KXX, 65P10

Key words: Lagrangian energy, extremals, discrete Euler-Lagrange equations

1 Single-time Lagrangian dynamics

Let $x \in R^n$ and let $\gamma = \{(t, x) | x = x(t), t_0 \leq t \leq t_1\}$ be a curve in the space $R \times R^n$. Let Γ be the set of all curves γ which join the point (t_0, x_0) , (t_1, x_1) . A differentiable function

$$L: R \times R^n \times R^n \rightarrow R$$

is called *Lagrangian density energy*.

Theorem 1.1 *A C^2 curve γ is an extremal of the functional*

$$E(\gamma) = \int_{t_0}^{t_1} L \left(t, x, \frac{dx}{dt} \right) dt, \quad \gamma \in \Gamma$$

iff it is a solution of Euler-Lagrange equations

$$\frac{\partial L}{\partial x^k} - \frac{d}{dt} \frac{\partial L}{\partial \left(\frac{dx^k}{dt} \right)} = 0, \quad k = 1, \dots, n.$$

This is a differential system of n equations of second order and therefore the solutions depend on $2n$ arbitrary constants. For fixing one solution there are used $2n$ boundary conditions

$$x(t_0) = x_0, \quad x(t_1) = x_1.$$

Since the property for γ to be an extremal of the functional E does not depend on the choice of the system of coordinates, the previous explanations extend easily to (Riemannian) manifolds.

The Lagrangian L produces the Hamiltonian

$$H(t, x, \dot{x}) = \dot{x}^i \frac{\partial L}{\partial \dot{x}^i}(t, x, \dot{x}) - L(t, x, \dot{x}),$$

which is conserved along the extremals only if it does not depend on the parameter t .

The discretization of L can be made by using the midpoint rule which consists in the substitution of t by h , of the point x with $\frac{x_{k+1} + x_k}{2}$, and of the velocity \dot{x} by $\frac{x_{k+1} - x_k}{h}$, where h is the time step. One obtains the discrete Lagrangian

$$L_d: R \times R^n \times R^n \rightarrow R, \quad L_d(h, u, v) = L\left(h, \frac{u+v}{2}, \frac{v-u}{h}\right).$$

This determines the action

$$S: R \times (R^n)^{N+1} \rightarrow R, \quad S(h; x_0, x_1, \dots, x_N) = \sum_{k=0}^{N-1} L_d(h, x_k, x_{k+1}), \quad x_k \in R^n.$$

The discrete variational principle characterizes the sequence $(x_0, x_1, \dots, x_N) \in (R^n)^{N+1}$ for which the action S is stationary, for any family $x_k(\varepsilon) \in R^n$, $\varepsilon \in I \subset R$, $0 \in I$, with $x_k(0) = x_k$, and x_0, x_N fixed points. Using the variation of the first order we find

Theorem 1.2 *The sequence (x_k) , $k = 0, 1, \dots, N$ is stationary for the action S iff it is generated by the discrete Euler-Lagrange equations (variational integrator)*

$$\frac{\partial L_d}{\partial x_k^i}(h, x_{k-1}, x_k) + \frac{\partial L_d}{\partial x_k^i}(h, x_k, x_{k+1}) = 0, \quad i = 1, \dots, n; \quad k = 1, \dots, N-1.$$

Denoting

$$A_i(k) = \frac{\partial L_d}{\partial x_k^i}(h, x_{k-1}, x_k), \quad f_i(u) = \frac{\partial L_d}{\partial x_k^i}(h, x_k, u) + A_i(k),$$

$$i = 1, \dots, n; \quad u = (u^1, \dots, u^n); \quad F = (f_1, \dots, f_n),$$

the preceding equations transfer into a nonlinear equation system

$$(1) \quad F(u) = 0,$$

at each step k . The solution of the system (1) can be approximated by using $u(e) = x_k$ in the Newton method

$$J_F(u(e)) \begin{pmatrix} u^1(e+1) \\ \dots \\ u^n(e+1) \end{pmatrix} = J_F(u(e)) \begin{pmatrix} u^1(e) \\ \dots \\ u^n(e) \end{pmatrix} - \begin{pmatrix} f_1(u(e)) \\ \dots \\ f_n(u(e)) \end{pmatrix},$$

$e = 1, 2, \dots, \bar{e}$. The matrix J_F is the Jacobi matrix of the function F , and the integer number \bar{e} is determined by the condition

$$\frac{\left| \sum_{i=1}^n f_i^2(u(e)) - \sum_{i=1}^n f_i^2(u(e+1)) \right|}{1 + \sum_{i=1}^n f_i^2(u(e+1))} < \varepsilon.$$

Next, we put $x_{k+1} = u(\bar{e})$.

The discrete Lagrangian L_d produces the discrete Hamiltonian

$$H_d(k) = \frac{x_k^i - x_{k-1}^i}{h} \frac{\partial L_d}{\partial \dot{x}^i}(h, x_{k-1}, x_k) - L_d(h, x_{k-1}, x_k).$$

2 Multi-time Lagrangian dynamics

In the preceding section the space coordinate and time played quite distinct roles: the space coordinate was merely an index numbering freedom degrees, and the time coordinate was the usual physical time in which the system evolves. According Dickey [1], such a theory is satisfactory unless we turn our attention to relativistic invariant equations, e.g. chiral fields, sine-Gordon, and others. Also considering the KP-hierarchy for arbitrary m and n , the variables x_m and x_n are quite equal in rights and there is no reason to prefer one to the other by choosing it as time. In such cases a new field theory is useful which involves many time variables. The multi-time formalism is of interest even for all examples where the variables are involved in a distinctly asymmetric way.

The multi-time calculus of variations is of course not new. Let $T_0 \subset R^p$ be a relatively compact domain. Let $\varphi = \{(t, x) | x = x(t), t \in T_0, x \in R^n\}$ be a parametrized sheet in the space $R^p \times R^n$. Let Φ be the set of all parametrized sheets φ satisfying the boundary condition $\varphi|_{\partial T_0} = f$, where f is a given continuous function. A differentiable function

$$L: R^p \times R^n \times R^{np} \rightarrow R$$

is called *Lagrangian density energy*.

Theorem 2.1 *A C^2 parametrized sheet is an extremal of the functional*

$$E(\varphi) = \int_{T_0} L \left(t^\alpha, x^i, \frac{\partial x^i}{\partial t^\alpha} \right) dt^1 \wedge \dots \wedge dt^p$$

iff it is a solution of Euler-Lagrange equations

$$\frac{\partial L}{\partial x^k} - \frac{\partial}{\partial t^\alpha} \frac{\partial L}{\partial x_\alpha^k} = 0, \quad x_\alpha^k = \frac{\partial x^k}{\partial t^\alpha}, \quad k = 1, \dots, n.$$

This is a PDEs system with n equations of second order. Therefore the solutions depend on $2n$ arbitrary functions. For fixing one solution we use the boundary condition.

Since the property of φ to be an extremal of the functional E does not depend on the choice of the system of coordinates, the previous explanations extend easily to Riemannian manifolds.

The Lagrangian L produces the Hamiltonian

$$H(t^\alpha, x^i, x_\alpha^i) = x_\beta^j \frac{\partial L}{\partial x_\beta^j}(t^\alpha, x^i, x_\alpha^i) - L(t^\alpha, x^i, x_\alpha^i),$$

but this function is not conserved along the extremals.

Suppose $p = 2$. The discretization of L can be made by using the *centroid rule* which consists in the substitution of the point t with the step (h_1, h_2) , of the point x with $\frac{x_{k\ell} + x_{k+1\ell} + x_{k\ell+1}}{3}$, and of partial velocities x_α , $\alpha = 1, 2$, by $\frac{x_{k+1\ell} - x_{k\ell}}{h_1}$, $\frac{x_{k\ell+1} - x_{k\ell}}{h_2}$. One obtains the discrete Lagrangian

$$L_d: R^2 \times R^n \times R^n \times R^n \rightarrow R, \quad L_d(u, v, w) = L\left(h_1, h_2, \frac{u+v+w}{3}, \frac{v-u}{h_1}, \frac{w-u}{h_2}\right).$$

This determines the 2-dimensional discrete action

$$S: R^2 \times (R^n)^{(M+1)(N+1)} \rightarrow R,$$

$$S(h_1, h_2; A) = \sum_{k=0}^{M-1} \sum_{\ell=0}^{N-1} L(h_1, h_2; x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}), \quad x_{k\ell} \in (R^n)^{(M+1)(N+1)},$$

$$A = \begin{pmatrix} x_{00} & x_{01} & \cdots & x_{0N} \\ x_{10} & x_{11} & \cdots & x_{1N} \\ \cdots & & & \\ x_{M0} & x_{M2} & \cdots & x_{MN} \end{pmatrix}.$$

We fix the 2-step (h_1, h_2) . The discrete variational principle consists in the characterization of the matrix A for which the action S is stationary, for any family $x_{k\ell}(\varepsilon) \in R^n$, $k \in \{0, 1, \dots, M-1\}$, $\ell \in \{0, 1, \dots, N-1\}$, $\varepsilon \in I \subset R$, $0 \in I$ with $x_{k\ell}(0) = x_{k\ell}$, and fixed lines $(x_{00}, x_{01}, \dots, x_{0N})$, $(x_{M0}, x_{M2}, \dots, x_{MN})$, fixed columns ${}^t(x_{00}, x_{10}, \dots, x_{M0})$, ${}^t(x_{0N}, x_{1N}, \dots, x_{MN})$. The discrete variational principle is obtained using the variation of S of the first order.

Theorem 2.2 *The first variation of the discrete action S is*

$$\begin{aligned} \delta S(A)(\eta) &= \frac{\partial L}{\partial x_{00}^i}(x_{00}, x_{10}, x_{01})\eta_{00}^i + \frac{\partial L}{\partial x_{10}^i}(x_{10}, x_{20}, x_{11})\eta_{10}^i + \frac{\partial L}{\partial x_{01}^i}(x_{01}, x_{11}, x_{02})\eta_{01}^i \\ &+ \sum_{k=1}^{M_1} \sum_{\ell=1}^{N-1} \left[\frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) + \frac{\partial L}{\partial x_{k\ell}^i}(x_{k-1\ell}, x_{k\ell}, x_{k-1\ell+1}) \right. \\ &+ \left. \frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell-1}, x_{k+1\ell-1}, x_{k\ell}) \right] \eta_{k\ell}^i + \sum_{k=1}^{M-1} \frac{\partial L}{\partial x_{k0}^i}(x_{k-10}, x_{k0}, x_{k-11})\eta_{k0}^i \\ &+ \sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x_{M\ell}^i}(x_{M-1\ell}, x_{M\ell}, x_{M-1\ell+1})\eta_{M\ell}^i + \sum_{\ell=1}^{N-1} \frac{\partial L}{\partial x_{0\ell}^i}(x_{0\ell-1}, x_{1\ell-1}, x_{0\ell})\eta_{0\ell}^i \\ &+ \sum_{k=0}^{M-1} \frac{\partial L}{\partial x_{kN}^i}(x_{kN-1}, x_{k+1N-1}, x_{kN})\eta_{kN}^i, \end{aligned}$$

where

$$\eta = \begin{pmatrix} \eta_{00} & \eta_{01} & \cdots & \eta_{0N} \\ \eta_{10} & \eta_{11} & \cdots & \eta_{1N} \\ \cdots & \cdots & \cdots & \cdots \\ \eta_{M0} & \eta_{M1} & \cdots & \eta_{MN} \end{pmatrix}, \quad \eta_{k\ell} = \left. \frac{\partial x_{k\ell}}{\partial \varepsilon} \right|_{\varepsilon=0},$$

$x_{k\ell}(\varepsilon) \in Q$, $\varepsilon \in I$, $0 \in I$, $x_{k\ell}(0) = x_{k\ell}$.

Proof. We use the family of curves $x_{k\ell}(\varepsilon) \in R^n$, $\varepsilon \in I$. Then

$$S(A(\varepsilon)) = \sum_{k=0}^{M-1} \sum_{\ell=0}^{N-1} L(x_{k\ell}(\varepsilon), x_{k+1\ell}(\varepsilon), x_{k\ell+1}(\varepsilon)).$$

We find

$$\begin{aligned} \delta S(A)(\eta) &= \left. \frac{\partial}{\partial \varepsilon} S(A(\varepsilon)) \right|_{\varepsilon=0} = \sum_{k=0}^{M-1} \sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) \eta_{k\ell}^i \\ &\quad + \sum_{k=0}^{M-1} \sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x_{k+1\ell}^i}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) \eta_{k+1\ell}^i \\ &\quad + \sum_{k=0}^{M-1} \sum_{\ell=0}^{N-1} \frac{\partial L}{\partial x_{k\ell+1}^i}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) \eta_{k\ell+1}^i. \end{aligned}$$

Corollary 2.1 (discrete Euler-Lagrange equations). *The matrix $A = (x_{k\ell})$ is stationary for the action S iff*

$$\begin{aligned} \frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) + \frac{\partial L}{\partial x_{k\ell}^i}(x_{k-1\ell}, x_{k\ell}, x_{k-1\ell+1}) + \frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell-1}, x_{k+1\ell-1}, x_{k\ell}) = 0, \\ i = 1, \dots, n; \quad k \in \{1, \dots, M-1\}, \quad \ell \in \{1, \dots, N-1\}. \end{aligned}$$

Proof. Since the boundary of the grid is fixed, the lines

$$(\eta_{00}, \eta_{01}, \dots, \eta_{0N}), \quad (\eta_{M0}, \eta_{M1}, \dots, \eta_{MN}),$$

and the columns

$${}^t(\eta_{00}, \eta_{10}, \dots, \eta_{M0}), \quad {}^t(\eta_{0N}, \eta_{1N}, \dots, \eta_{MN})$$

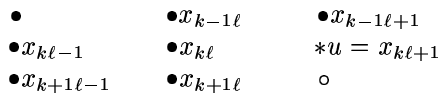
must be zero, and $\eta_{k\ell}$, $k \in \{1, \dots, M-1\}$, $\ell \in \{1, \dots, N-1\}$ are arbitrary.

The variational integrator described by the discrete Euler-Lagrange equations works as follows:

- we give the lines $(x_{00}, x_{01}, \dots, x_{0N})$, $(x_{10}, x_{11}, \dots, x_{1N})$;
- we denote

$$\begin{aligned} u &= x_{k\ell+1}, \\ A_i(k\ell) &= \frac{\partial L}{\partial x_{k\ell}^i}(x_{k-1\ell}, x_{k\ell}, x_{k-1\ell+1}), \quad B_i(k\ell) = \frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell-1}, x_{k+1\ell-1}, x_{k\ell}), \\ f_i(u) &= \frac{\partial L}{\partial x_{k\ell}^i}(x_{k\ell}, x_{k+1\ell}, u) + A_i(k\ell) + B_i(k\ell), \quad F = (f_1, \dots, f_n); \end{aligned}$$

- we solve the nonlinear system (4) $F(u) = 0$, at each step (k, ℓ) using six points of starting as shown a part of the grid,



Newton Method

The solution of the nonlinear system (4) can be approximated by using $u(\ell) = x_{k\ell+1}$ in the Newton method

$$J_F(u(e)) \begin{pmatrix} u^1(e+1) \\ \vdots \\ u^n(e+1) \end{pmatrix} = J_F(u(e)) \begin{pmatrix} u^1(e) \\ \vdots \\ u^n(e) \end{pmatrix} - \begin{pmatrix} f_1(u(e)) \\ \vdots \\ f_n(u(e)) \end{pmatrix},$$

$e = 1, 2, \dots, \bar{e}$. The matrix J_F is the Jacobi matrix of the function F , and the integer \bar{e} is determined by the condition

$$\frac{\left| \sum_{i=1}^n f_i^2(u(e)) - \sum_{i=1}^n f_i^2(u(e+1)) \right|}{1 + \sum_{i=1}^n f_i^2(u(e+1))} < \varepsilon.$$

Next, we put $x_{k\ell+2} = u(\bar{e})$.

The discrete Lagrangian L_d produces the discrete Hamiltonian

$$\begin{aligned}
 H_d(k, \ell) &= \frac{x_{k+1\ell}^i - x_{k\ell}^i}{h_1} \frac{\partial L}{\partial x_1^i} (h_1, h_2, x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) \\
 &+ \frac{x_{k\ell+1}^i - x_{k\ell}^i}{h_2} \frac{\partial L}{\partial x_2^i} (h_1, h_2, x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}) - L_d (h_1, h_2, x_{k\ell}, x_{k+1\ell}, x_{k\ell+1}).
 \end{aligned}$$

Acknowledgements. A version of this paper was presented by the first two authors at the third Conference of Balkan Society of Geometers, Workshop on Electromagnetic Flows and Dynamics, July 31-August 3, 2000, University POLITEHNICA of Bucharest, Romania.

References

- [1] L.A. Dickey: Soliton equations and Hamiltonian systems, *Advanced Series in Mathematical Physics*, Vol. 12, World Scientific Publishing, Singapore, 1991.
- [2] H.Y. Guo, Y.Q. Li, K. Wu and S.K. Wang: Difference discrete variational principle, Euler-Lagrange cohomology and symplectic, multisymplectic structures, arXiv:math-ph/0106001 v1 1 Jun 2001.
- [3] D. Opreș and C. Giulvezan: *Geometric Integrators and Applications*, Mirton Publishing House, Timișoara, 1999 (in Romanian).

- [4] C. Udriște: Electromagnetic dynamical systems and new variants of Lorentz law, Research Grant, University Politehnica of Bucharest-Ministry of National Education, 1998-2001.
- [5] C. Udriște and M. Postolache: Least squares problem and geometric dynamics, *Ital. J. Pure Appl. Math.*, **15** (2000) (in printing).
- [6] C. Udriște and M. Postolache: Least squares problem and magnetic dynamics, in *Global Analysis, Differential Geometry and Lie Algebras* (Gr. Tsagas (Ed.)); Workshop on Global Analysis, Differential Geometry and Lie Algebras, Thessaloniki, June 24-28 (2000); pp. 169-238, 2000.
- [7] C. Udriște: *Geometric Dynamics*, Southeast Asian Bulletin of Mathematics, Springer-Verlag 24 (2000), 313-322; Kluwer Academic Publishers, Dordrecht/Boston/London, Mathematics and Its Applications, 513, 2000.
- [8] C. Udriște: Multi-time dynamics induced by 1-forms and metrics, in *Global Analysis, Differential Geometry and Lie Algebras*, BSG Proceedings 5, Ed. Grigorios Tsagas, Geometry Balkan Press (2001), 169-178.
- [9] C. Udriște and M. Postolache: *Atlas of Magnetic Dynamics*, Geometry Balkan Press, 2001.

Politehnica University of Bucharest
Department of Mathematics I
Splaiul Independenței 313, 77206 Bucharest, Romania
E-mail:udriste@mathem.pub.ro