LAGRANGIAN INTEGRATION WITH SYMPLECTIC METHODS

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Abstract. In this short note we show how to obtain Lagrangian integrators from known symplectic partitioned Runge-Kutta methods.

Key words. Euler-Lagrange equations, Hamiltonian system, Lagrangian system, partitioned Runge-Kutta method, symplecticness

AMS subject classifications. 65L05, 65L06, 70H05, 70H35

1. Introduction. Lagrangian systems are fundamental in one of the most important field of mathematics: the calculus of variations [3]. The main motivation of this short note is to seek numerical integrators preserving the variational character of the solutions to Lagrangian systems, which is certainly of great interest. They are called *Lagrangian integrators*. To our knowledge, only one second-order Lagrangian integrator has been proposed in the literature [9]. In this note it is shown that under certain conditions the numerical solution of a Lagrangian system by an unusual application of symplectic partitioned Runge-Kutta methods can be interpreted as the exact solution of a perturbed Lagrangian system, thus is a Lagrangian integrator.

2. Lagrangian and Hamiltonian systems. We give briefly some definitions and theoretical results related to Lagrangian and Hamiltonian systems [1, 2, 9]. For a function $f(x,y)$, we denote by $f_x(x,y)$ its partial derivative with respect to x.

Let $L(q,v,t) : \mathbf{R}^n \times \mathbf{R}^n \times \mathbf{R} \mapsto \mathbf{R}$ be a twice differentiable function called the *Lagrangian*. The *energy* function with respect to the Lagrangian L is defined by

$$E(q,v,t) := L_v(q,v,t)v - L(q,v,t) \ . \tag{1}$$

Lagrangian systems arise for example in classical mechanics where the Lagrangian is decomposed as $L = T - U$, where $T(q,v) = \frac{1}{2} v^T M(q) v$ is the kinetic energy with $M(q)$ a strictly positive definite symmetric mass matrix, and $U(q,v,t)$ is the generalized potential energy. The energy function (1) is given in this situation by

$$E(q,v,t) = T(q,v) + U(q,v,t) - U_v(q,v,t)v \ .$$

Let $q(t) : \mathbf{R} \mapsto \mathbf{R}^n$ be a differentiable function. The *action*, also called the *fundamental integral*, with respect to the Lagrangian L and the function $q(t)$ is defined by

$$S(q) := \int_{t_0}^{t_1} L(q(t), \dot{q}(t), t) dt \ .$$

A *stationary solution* of the action is a function $q(t)$ such that the first variation of the action satisfies $\delta S(q) = 0$. In this case the action $S(q)$ is called a *Lagrangian action*. Stationary solutions can be characterized as follows:

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THEOREM 2.1. *The function $q(t)$ is a stationary solution of the action S if and only if $q(t)$ satisfies the* Euler-Lagrange equations, *also called the* Lagrangian system,

$$\dot{q} = v \ , \qquad \frac{d}{dt} L_v^T(q,v,t) = L_q^T(q,v,t) \ . \tag{2}$$

Moreover, we have

$$\frac{d}{dt} E(q(t),v(t),t) = -L_t(q(t),v(t),t) \ .$$

Hence, if L is independent of t then the energy is constant.

THEOREM 2.2. *If $q(t)$ is an extremum of the action S then it is necessarily a stationary solution.*

There is a close connection between Lagrangian and Hamiltonian systems. The *momenta* of a Lagrangian system are defined by

$$p := L_v^T(q,v,t) \ . \tag{3}$$

Assuming that

$$L_{vv}(q,v,t) \text{ is strictly positive definite} \ , \tag{4}$$

thus invertible, this ensures existence and uniqueness of a solution to the Euler-Lagrange equations (2) given initial values (q_0, v_0, t_0). Under the assumption (4), the relation (3) also defines v as an implicit function $v(q,p,t)$. The Legendre transformation of the Lagrangian $L(q,v,t)$ with respect to v is then given by

$$H(q,p,t) := p^T v - L(q,v,t) \ . \tag{5}$$

The function H is called the *Hamiltonian*. Because of

$$v = H_p^T(q,p,t) \ , \tag{6}$$

we have $H_{pp} = L_{vv}^{-1}$ and the assumption (4) is equivalent to

$$H_{pp}(q,p,t) \text{ is strictly positive definite} \ , \tag{7}$$

i.e., the Hamiltonian is *optical* [9]. It can be easily seen that the Legendre transformation of the Hamiltonian $H(q,p,t)$ with respect to p is nothing else but the Lagrangian $L(q,v,t)$. A close relation between Hamiltonian and Lagrangian systems is stated precisely in the following theorem:

THEOREM 2.3. *Under the assumption (4) the Lagrangian system (2) is equivalent by the change of variables (3) and the Legendre transformation (5) to the* Hamiltonian system

$$\dot{q} = H_p^T(q,p,t) \ , \qquad \dot{p} = -H_q^T(q,p,t) \ . \tag{8}$$

Hence, we have

$$\frac{d}{dt} H(q(t),p(t),t) = H_t(q(t),p(t),t) = -L_t(q(t),v(t),t) = \frac{d}{dt} E(q(t),v(t),t) \ . \tag{9}$$

Conversely, under the assumption (7) the Hamiltonian system (8) is equivalent by the change of variables (6) and the Legendre transformation (5) to the Lagrangian system (2), and (9) holds.

The main property of the flow $\phi_\tau : (q(t), p(t)) \mapsto (q(t+\tau), p(t+\tau))$ of Hamiltonian systems (8) is that of *symplecticness*, i.e.,

$$\text{(10)} \qquad \text{the 2-form } dq \wedge dp = \sum_{i=1}^{n} dq_i \wedge dp_i \text{ is preserved by the flow } \phi_\tau \ .$$

This property can be transfered under the assumption (4) to the flow $\psi_\tau : (q(t), v(t)) \mapsto (q(t+\tau), v(t+\tau))$ of Lagrangian systems, i.e.,

$$\text{the 2-form } dq \wedge dL_v^T(q,v,t) = \sum_{i=1}^{n} dq_i \wedge (dL_v)_i(q,v,t) \text{ is preserved by the flow } \psi_\tau \ .$$

3. Symplectic partitioned Runge-Kutta methods. The application to the Hamiltonian system (8) of one step of an s-stage *partitioned Runge-Kutta (PRK)* method with coefficients (b_i, a_{ij}, c_i)-$(\widehat{b}_i, \widehat{a}_{ij}, c_i)$, initial values (q_0, p_0, t_0), and stepsize h reads

$$\text{(11a)} \qquad Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} H_p^T(Q_j, P_j, t_0 + c_j h) \ ,$$

$$\text{(11b)} \qquad P_i = p_0 - h \sum_{j=1}^{s} \widehat{a}_{ij} H_q^T(Q_j, P_j, t_0 + c_j h) \ ,$$

$$\text{(11c)} \qquad q_1 = q_0 + h \sum_{i=1}^{s} b_i H_p^T(Q_i, P_i, t_0 + c_i h) \ ,$$

$$\text{(11d)} \qquad p_1 = p_0 - h \sum_{i=1}^{s} \widehat{b}_i H_q^T(Q_i, P_i, t_0 + c_i h) \ .$$

PRK methods for which the local numerical flow preserves the property of symplecticness (10) are characterized as follows:

THEOREM 3.1. *[10] If the PRK method (11) applied to the Hamiltonian system (8) satisfies*

$$\text{(12a)} \qquad b_i = \widehat{b}_i \quad i = 1, \ldots, s \ ,$$

$$\text{(12b)} \qquad b_i \widehat{a}_{ij} + \widehat{b}_j a_{ji} - b_i \widehat{b}_j = 0 \quad i, j = 1, \ldots, s \ ,$$

then the numerical flow $(q_0, p_0) \mapsto (q_1, p_1)$ is symplectic. For irreducible PRK methods the conditions (12) are also necessary for symplecticness.

The main motivation for the use of symplectic PRK methods lies in the following backward error result:

THEOREM 3.2. *[4] Consider a PRK method (11) of order r satisfying the conditions (12) (symplectic) and assume that the Hamiltonian function $H(q,p,t)$ is $(N+1)$-times continuously differentiable. Then the numerical solution (q_1, p_1) satisfies*

$$q_1 = \widetilde{q}(t_0 + h) + O(h^{N+1}) \ , \qquad p_1 = \widetilde{p}(t_0 + h) + O(h^{N+1})$$

where $(\widetilde{q}(t), \widetilde{p}(t))$ is the exact solution of a perturbed Hamiltonian system

$$\dot{\widetilde{q}} = \widetilde{H}_p^T(\widetilde{q}, \widetilde{p}, t) \ , \qquad \dot{\widetilde{p}} = -\widetilde{H}_q^T(\widetilde{q}, \widetilde{p}, t)$$

with Hamiltonian $\widetilde{H} = H + h^r H_r + h^{r+1} H_{r+1} + \ldots + h^{N-1} H_{N-1}$. The H_i are called the elementary Hamiltonians.

This is a very fundamental result, since we can infer that the numerical flow of a symplectic method at constant stepsizes is a global symplectic transformation.

4. Lagrangian integrators. We show that similar results to those derived in the previous section hold for Lagrangian systems. Under the assumption (4), by Theorem 2.3 the Lagrangian system (2) can be reformulated in terms of an equivalent Hamiltonian system (8) with variables (q,p). A PRK method can be formally applied to this Hamiltonian system and then be rewritten in terms of the variables (q,v) of the Lagrangian form. This leads to the following unusual application of PRK methods to the Lagrangian system (2)

$$Q_i = q_0 + h\sum_{j=1}^{s} a_{ij} V_j \ , \tag{13a}$$

$$L_v^T(Q_i,V_i,t_0+c_ih) = L_v^T(q_0,v_0,t_0) + h\sum_{j=1}^{s} \widehat{a}_{ij} L_q^T(Q_j,V_j,t_0+c_jh) \ , \tag{13b}$$

$$q_1 = q_0 + h\sum_{i=1}^{s} b_i V_i \ , \tag{13c}$$

$$L_v^T(q_1,v_1,t_0+h) = L_v^T(q_0,v_0,t_0) + h\sum_{i=1}^{s} \widehat{b}_i L_q^T(Q_i,V_i,t_0+c_ih) \ . \tag{13d}$$

For h sufficiently small, existence and uniqueness of the PRK solution (q_1,v_1) holds under the assumption (4) by the implicit function theorem. A similar application of PRK methods has been proposed for the numerical solution of mechanical systems in [7]. For such systems the equations are given by

$$\dot{q} = v \ , \qquad M(q)\dot{v} = f(q,v)$$

where $M(q)$ is the symmetric generalized mass matrix and $f(q,v)$ is the vector of generalized forces. The generalized forces $f(q,v)$ contain the term

$$-M_q(q)(v,v)$$

which is referred to as the Coriolis forces. Therefore, using instead the formulation

$$\frac{d}{dt}(M(q)v) = M_q(q)(v,v) + f(q,v)$$

is advantageous since the Coriolis forces then cancel out.

A direct consequence of Theorem 3.1 is:

THEOREM 4.1. *Under the assumption (4), if the PRK method (13) applied to the Lagrangian system (2) satisfies (12) then the transformation* $(q_0, L_v^T(q_0,v_0,t_0)) \mapsto (q_1, L_v^T(q_1,v_1,t_0+h))$ *preserves the* 2*-form* $dq \wedge dL_v^T(q,v,t)$. *For irreducible PRK methods these conditions (12) are also necessary to preserve this* 2*-form.*

In terms of the variables (q,p) of the Hamiltonian the numerical solution of a PRK method satisfying the conditions (12) (symplectic) can be interpreted by Theorem 3.2 as the exact solution (up to a certain truncation error) of a perturbed Hamiltonian system. Using the relations (6) and (5), this perturbed Hamiltonian $\widetilde{H}(\widetilde{q},\widetilde{p},t)$ defines a perturbed Lagrangian $\widetilde{L}(\widetilde{q},\widetilde{v},t)$ (and also a perturbed energy $\widetilde{E}(\widetilde{q},\widetilde{v},t) = \widetilde{H}(\widetilde{q},\widetilde{p}(\widetilde{q},\widetilde{v},t),t)$). Hence, we can now state:

THEOREM 4.2. *Consider a PRK method (13) of order* r *satisfying the conditions (12) (symplectic) and assume that the Lagrangian function* $L(q,v,t)$ *satisfies (4) and*

is $(N+1)$-times continuously differentiable. Then the numerical solution (q_1, v_1) satisfies

$$q_1 = \widetilde{q}(t_0+h) + O(h^{N+1}) \ , \qquad v_1 = \widetilde{v}(t_0+h) + O(h^{N+1})$$

where $(\widetilde{q}(t), \widetilde{v}(t))$ is the exact solution of a perturbed Lagrangian system

$$\dot{\widetilde{q}} = \widetilde{v} \ , \qquad \frac{d}{dt}\widetilde{L}_v^T(\widetilde{q},\widetilde{v},t) = \widetilde{L}_q^T(\widetilde{q},\widetilde{v},t) \ .$$

with Lagrangian $\widetilde{L} = L + h^r L_r + h^{r+1} L_{r+1} + \ldots + h^{N-1} L_{N-1}$.

As a direct consequence of this theorem we obtain the main result of this note:

COROLLARY 4.3. *In addition to the hypotheses of Theorem 4.2 suppose that the action S with respect to the Lagrangian L admits an extremum. Then the numerical approximation of this extremum by a PRK method satisfying the conditions (12) (symplectic) is an extremum (up to a certain truncation error $O(h^{N+1})$) of the action S with respect to a perturbed Lagrangian.*

Examples of Lagrangian integrators (13) are thus given by the Gauss RK family [5, 6] and the Lobatto IIIA-IIIB PRK family [8] from which the familiar Verlet-leapfrop algorithm is the simplest member [11]. The above results can in fact be extended to any symplectic integrator provided that it can be applied directly to Lagrangian systems and that a backward error result similar to Theorem 3.2 holds.

5. A numerical experiment. As a numerical illustration, we consider the Euler-Lagrange equations for the spherical pendulum in angular coordinates with unit mass and gravity. The Lagrangian is given by $L = T - U$ where the kinetic energy is $T = \frac{1}{2}(\dot{\theta}^2 + \sin^2(\theta)\dot{\varphi}^2)$ and the potential energy is $U = -\cos(\theta)$. We have applied to this system the three-stage fourth-order Lobatto IIIA-IIIB PRK method as specified in (13) with stepsize $h = 0.02$. The initial values used are $\theta_0 = 0$, $\phi_0 = 0.17$, $\dot{\theta}_0 = 1$, $\dot{\phi}_0 = 0$. In Fig. 1 we have plotted the energy error versus time. We clearly observe that the energy error remains bounded which is a demonstration of the variational character of the integrator. Moreover, since $L_\varphi = 0$ the quantity $L_{\dot{\varphi}} = \sin^2(\theta)\dot{\varphi}$ is constant (Kepler's second law) and is preserved exactly up to the machine precision.

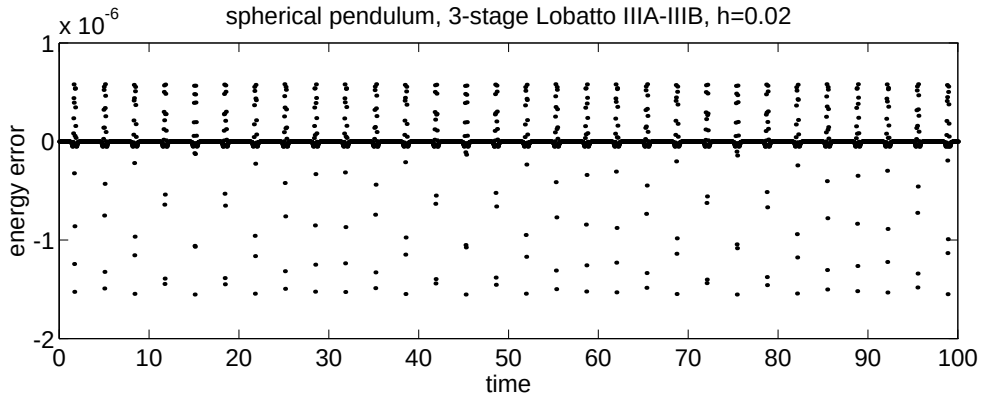

FIG. 1. *Energy error for the spherical pendulum using the three-stage Lobatto IIIA-IIIB.*

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