

On the Γ -Convergence of Discrete Dynamics and Variational Integrators

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Summary. For a simple class of Lagrangians and variational integrators, derived by time discretization of the action functional, we establish (i) the Γ -convergence of the discrete action sum to the action functional; (ii) the relation between Γ -convergence and weak* convergence of the discrete trajectories in $W^{1,\infty}(\mathbb{R}; \mathbb{R}^n)$; and (iii) the relation between Γ -convergence and the convergence of the Fourier transform of the discrete trajectories as measured in the flat norm.

Key words. discrete dynamics, variational integrators, Γ -convergence, spectral convergence, flat norm

1. Introduction

This work is concerned with the application of Γ -convergence methods to the elucidation of the convergence properties of discrete dynamics and variational integrators. The theory of *discrete dynamics* has a relatively short but vigorous history. A recent review of this history may be found in [10], which can also be consulted for an up-to-date review of the subject. As understood here, discrete dynamics is a theory of Lagrangian mechanics in which time is regarded as a discrete variable *ab initio*, and in which the discrete trajectories follow from a discrete version of Hamilton's principle, obtained by replacing the action integral by an action sum. The mechanical properties of the discrete system are described by a discrete Lagrangian, defined as a function of pairs of points in configuration space. Using generating functions, Veselov [13] (see also [11]) showed that the discrete Euler-Lagrange equations generate symplectic maps. Wendlandt and Marsden [14] pointed out that Veselov's theory of discrete dynamics can be used to formulate

numerical methods for time integration of Lagrangian systems, known as *variational integrators*. Wendlandt and Marsden [14] also showed that variational integrators are automatically symplectic and conserve discrete momentum maps, such as linear and angular momentum, exactly along discrete trajectories. By adopting a spacetime view of Lagrangian mechanics, as advocated by Marsden et al. [9], it is possible to devise variational integrators which preserve the energy, momentum, and symplectic structure, as shown by Kane et al. [7]. Extensions of the theory to partial differential equations based on multisymplectic geometry may be found in [9].

The convergence properties of variational integrators have been ascertained using conventional techniques, such as Gronwall's inequality [10], or by backward error analysis [5], [12], [10]. In addition, time-stepping algorithms for linear structural dynamics have also been traditionally analyzed by *phase-error analysis* [1], [2], [6].

The elementary example of the harmonic oscillator may conveniently be used to motivate the approach developed in this paper. The action integral of an unforced harmonic oscillator of mass $m > 0$ and stiffness $C > 0$ over the time interval (a, b) is

$$I(u, (a, b)) = \int_a^b ((m/2)\dot{u}^2(t) - (C/2)u^2(t)) dt, \quad (1.1)$$

where t denotes time, u the generalized coordinate of the oscillator, and here and subsequently, a superposed dot denotes time differentiation. The Euler-Lagrange equation of this system is

$$m\ddot{u} + Cu = 0, \quad (1.2)$$

and the general solution of this equation is

$$u(t) = \Re A_0 e^{i\omega_0 t}, \quad (1.3)$$

where $\omega_0 = \sqrt{C/m}$ is the natural frequency of the oscillator. The complex amplitude A_0 may be parameterized in terms of initial data, e.g.,

$$\Re A_0 = u(0), \quad \Im A_0 = -\frac{\dot{u}(0)}{\omega_0} = -\frac{p(0)}{m\omega_0}, \quad (1.4)$$

where $p = m\dot{u}$ is the linear momentum of the oscillator. The general solution (1.3) can also be characterized by its Fourier transform

$$\hat{u}(\omega) = \int_{-\infty}^{\infty} u(t) e^{-i\omega t} dt = A_0 \delta(\omega - \omega_0). \quad (1.5)$$

It is important to note that $\hat{u}(\omega)$ consists of a Dirac-delta function concentrated at ω_0 .

Consider now a partition $a = t_0 < t_1 = t_0 + h < \dots < t_k < t_{k+1} = t_k + h < \dots < t_N = b$. In the theory of discrete dynamics (e.g., [10]), the discrete trajectories follow as the stationary points of the discrete action

$$I_h(u, (a, b)) = \sum_{k=0}^{N-1} L_d(u_k, u_{k+1}), \quad (1.6)$$

where $u_k = u(t_k)$ and the discrete Lagrangian $L_d(u_k, u_{k+1})$ approximates the action $I(u, (t_k, t_{k+1}))$. A simple discrete Lagrangian for the harmonic oscillator is

$$L_d(u_k, u_{k+1}) = \frac{m}{2} \frac{(u_{k+1} - u_k)^2}{h} - h \frac{C}{2} u_k^2. \quad (1.7)$$

The corresponding linear momentum is

$$p_k = \frac{\partial L_d}{\partial u_k}(u_k, u_{k+1}) = m \frac{u_k - u_{k+1}}{h}, \quad (1.8)$$

and the discrete Euler-Lagrange equation is

$$m \frac{u_{k+1} - 2u_k + u_{k-1}}{h} + hCu_k = 0, \quad (1.9)$$

which is also the result of applying the central difference scheme to (1.2). A trite calculation shows that the general solution of this equation is

$$u_k = \Re A_h e^{i\omega_h t_k} \quad (1.10)$$

for some discrete amplitude A_h and frequency

$$\omega_h = \frac{1}{h} \arccos \left(1 - \frac{\omega_0^2 h^2}{2} \right). \quad (1.11)$$

As before, the amplitude can be parameterized in terms of initial data which, in view of (1.8), leads to the relations

$$\Re A_h = u(0), \quad \Im A_h = \frac{hp(0)/m - u(0)(1 - \cos \omega_h h)}{\sin \omega_h h}. \quad (1.12)$$

The general discrete solution (1.10) can also be characterized by its discrete Fourier transform

$$\hat{u}_h(\omega) = h \sum_{k \in \mathbb{Z}} u_k e^{-i\omega k h} = A_h \delta(\omega - \omega_h). \quad (1.13)$$

We note that $\hat{u}_h(\omega)$ again consists of a Dirac-delta function concentrated at ω_h .

It is evident from (1.10), (1.11), and (1.12) that, for given initial data, $A_h \neq A$ and $\omega_h \neq \omega$. Thus time-discretization schemes that, as exemplified by the central differences scheme, result in oscillatory solutions introduce two types of errors: *amplitude* errors and frequency or *phase* errors. We note in addition that, for the central differences scheme, we have

$$\lim_{h \rightarrow 0} \omega_h = \omega_0, \quad (1.14a)$$

$$\lim_{h \rightarrow 0} A_h = A_0, \quad (1.14b)$$

i.e., the discrete frequency and amplitude converge to the corresponding continuous-time limits as the time step h becomes vanishingly small. This is a natural notion of

convergence that forms the basis of the traditional *phase-error analysis* of time-stepping algorithms for linear structural dynamics [1], [2], [6]. In this type of analysis, the focus is in establishing the convergence of the amplitude and frequency of oscillatory numerical solutions to the amplitude and frequency of the exact solution, a form of convergence which we shall refer to as *spectral convergence*. Phase-error analysis is a particularly powerful tool inasmuch as it establishes the convergence of solutions in a global, instead of merely local, sense. In particular, it allows to compare infinite wave trains. This is in analogy to backward-error analysis [5], [12], [10], which is also global in nature, and in contrast to other conventional methods of analysis, such as Gronwall's inequality [10], that merely provide local exponential bounds on discretization errors.

The engineering literature on the subject of phase-error analysis relies on a case-by-case analysis of linear time-stepping algorithms, and general conditions ensuring spectral convergence do not appear to have been known, nor do extensions of phase-error analysis to nonlinear systems appear to be in existence. A hint as to how these extensions may be attempted is again provided by the simple harmonic oscillator example discussed above. We recall that the flat norm (cf. Section 3 for a brief review) supplies a natural distance between Dirac deltas of differing amplitudes and supports. Thus the convergence of $A_h \delta(\omega - \omega_h)$ to $A_0 \delta(\omega - \omega_0)$ in the flat norm is equivalent to the convergence of $A_h \rightarrow A_0$ and $\omega_h \rightarrow \omega_0$. It is therefore natural to investigate conditions ensuring the convergence of the Fourier transform of the discrete trajectories as measures in the flat norm.

Another natural—and seemingly unrelated—notion of convergence for discrete dynamics is Γ -convergence. Indeed, the variational character of variational integrators opens the way for the application of Γ -convergence methods to the problem of understanding the convergence properties of discrete dynamics, a line of inquiry that appears not to have been pursued to date. The Γ -convergence of functionals, introduced by De Giorgi and Franzoni [4] is a variational notion of convergence. It is a very versatile tool, and it implies convergence of minimizers under rather general conditions. In the present context, however, there seem to be two obstacles to bringing Γ -convergence to bear. First, stationary points of the action functional are typically not minimizers and Γ -convergence in general provides no information about nonminimizing stationary points. Secondly, we are interested in solutions on the entire real line such as infinite wave trains, and global variational methods such as Γ -convergence suffer from the fact that the functional is $+\infty$ or $-\infty$ on most trajectories. In this paper we point out how these difficulties can be overcome. We focus on a simple class of Lagrangians and establish

- (i) The Γ -convergence of the discrete action sum to the action functional.
- (ii) The relation between Γ -convergence of the discrete action sum and weak* convergence of the discrete trajectories in $W^{1,\infty}(\mathbb{R}; \mathbb{R}^n)$.
- (iii) The relation between Γ -convergence of the discrete action sum and the convergence of the Fourier transform of the discrete trajectories as measured in the flat norm.

It bears emphasis that these notions of convergence are not local, as are those derived from consistency and Gronwall's inequality, but apply to infinite wave trains. In particular, (iii) forges a connection between phase-error analysis and spectral convergence, and extends the former to nonlinear systems.

Although we focus in this paper on a simple class of Lagrangians to keep the resulting calculations simple (and sometimes elementary), we would like to emphasize that the Γ -convergence framework is very flexible and allows for many extensions. In fact, based on our work, Maggi and Morini [8] have recently studied much more general Lagrangians.

2. Formulation of the Problem

To study problems on the entire real line, we work with functions that are locally in L^2 , i.e., they are square-integrable on each bounded open interval. We set $X = L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$, and let \mathcal{E} be the collection of all open bounded intervals of \mathbb{R} . We recall that the space $L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$ can naturally be equipped with a countable system of seminorms $\|u\|_{L^2_{\text{loc}}(A_k, \mathbb{R}^n)}$, where A_k is an increasing sequence of open bounded intervals such that $\cup_k A_k = \mathbb{R}$. These seminorms define a distance with respect to that $L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$ becomes a complete metric space. In the same way we define the Sobolev space H^1_{loc} , which consists of functions that are in L^2_{loc} together with their first derivatives. By C^∞_c we denote the space of smooth functions with compact support.

Let $m > 0$ and $V \in C(\mathbb{R}^n)$. The functional $I : X \times \mathcal{E} \rightarrow \mathbb{R}$ defined by

$$I(u, A) = \begin{cases} \int_A \left(\frac{m}{2} |\dot{u}(t)|^2 - V(u(t)) \right) dt, & u \in H^1(A, \mathbb{R}^n), \\ +\infty, & \text{otherwise,} \end{cases} \quad (2.1)$$

is the action of u over the open bounded interval A . If $V \in C^1$, the first variation of I is the functional $\delta I : H^1_{\text{loc}}(\mathbb{R}, \mathbb{R}^n) \times C^\infty_c(\mathbb{R}, \mathbb{R}^n) \times \mathcal{E} \rightarrow \mathbb{R}$ defined by

$$\delta I(u, \varphi, A) = \int_A (m \dot{u}(t) \dot{\varphi}(t) - DV(u(t)) \varphi(t)) dt. \quad (2.2)$$

The stationary points of I are functions u such that

$$I(u, A) < \infty, \quad \delta I(u, \varphi, A) = 0, \quad \forall A \in \mathcal{E}, \varphi \in C^\infty_c(A, \mathbb{R}^n). \quad (2.3)$$

One important ingredient in our variational approach is that stationary points are minimizers when restricted to sufficiently short intervals. In fact, for sufficiently short intervals and fixed Dirichlet conditions the functional becomes convex (even though $-V$ may be nonconvex), and this simplifies the subsequent analysis.

Lemma 2.1. *Let u be a stationary point of the action functional (2.1). Assume in addition that V is C^2 and that there is a constant $C > 0$ such that $|D^2V| \leq C$. Let $a < b$ be such that $b - a < \pi/\omega_0$ with $\omega_0 = \sqrt{C/m}$. Then u minimizes $I(\cdot, (a, b))$ among all functions $v \in X$ with $v(a) = u(a)$, $v(b) = u(b)$, where $v(a)$ is understood as the left-sided limit and $v(b)$ is understood as the right-sided limit.*

Remark 2.2. A generic function $v \in X$ is only defined up to sets of measure zero. Hence the value $v(a)$ may not be defined. For the purpose of minimizers, however, it suffices to consider functions with $I(v, A) < \infty$. Then $v|_{(a,b)} \in H^1((a, b), \mathbb{R}^n)$ and hence the one-sided limits $v(a)$ and $v(b)$ exist in view of the Sobolev embedding theorem.

Proof. Let $\varphi \in C_c^\infty((a, b), \mathbb{R}^n)$. Then

$$\begin{aligned} I(u + \varphi, (a, b)) - I(u, (a, b)) \\ = \delta I(u, \varphi, (a, b)) \\ + \int_a^b \left(\frac{m}{2} \dot{\varphi}^2(t) - V(u(t) + \varphi(t)) + V(u(t)) + DV(u(t)) \cdot \varphi(t) \right) dt. \end{aligned} \quad (2.4)$$

But u is a stationary point of I and, hence, $\delta I(u, \varphi, (a, b)) = 0$. Therefore

$$\begin{aligned} I(u + \varphi, (a, b)) - I(u, (a, b)) \\ = \int_a^b \left(\frac{m}{2} \dot{\varphi}^2(t) - V(u(t) + \varphi(t)) + V(u(t)) + DV(u(t)) \cdot \varphi(t) \right) dt. \end{aligned} \quad (2.5)$$

But by Taylor's theorem we have

$$|V(u + \varphi) - V(u) - DV(u)\varphi|(x) = \frac{1}{2} |D^2V(u(x) + \lambda(x)\varphi(x))| |\varphi(x)|^2, \quad (2.6)$$

for some $\lambda(x) \in [0, 1]$. In addition, by the assumed upper bound on $|D^2V|$, we have

$$|V(u + \varphi) - V(u) - DV(u)\varphi| \leq \frac{C}{2} |\varphi|^2, \quad (2.7)$$

and

$$\begin{aligned} I(u + \varphi, (a, b)) - I(u, (a, b)) &\geq \int_a^b \left(\frac{m}{2} \dot{\varphi}^2 - \frac{C}{2} |\varphi|^2 \right) dt \\ &\geq \left(\frac{m}{2} \frac{\pi^2}{(b-a)^2} - \frac{C}{2} \right) \int_a^b |\varphi|^2 dt, \end{aligned} \quad (2.8)$$

where we have made use of Poincaré's inequality. Clearly, the right-hand side of this inequality is strictly positive provided that

$$\frac{m}{2} \frac{\pi^2}{(b-a)^2} - \frac{C}{2} > 0, \quad (2.9)$$

which in turn holds if $b - a < \pi/\sqrt{C/m}$. By a density estimate (2.8) holds also for functions in $H_0^1((a, b), \mathbb{R}^n)$. Hence we may take $\varphi = v - u$, and the proof is finished. \square

3. The Flat Norm on Measures

Definition 3.1. Let μ be a Radon measure on \mathbb{R}^n . Then the flat norm of μ is

$$\|\mu\| = \sup \left\{ \int_{\mathbb{R}^n} f d\mu \mid f : \mathbb{R} \rightarrow \mathbb{R} \text{ Lipschitz, } \text{Lip } f \leq 1, \sup |f| \leq 1 \right\}. \quad (3.1)$$

As a direct consequence of the definition, one obtains

$$\|\delta_a\| = 1, \quad \|\delta_a - \delta_b\| = \min(|a - b|, 2). \quad (3.2)$$

We will apply the flat norms to measures in Fourier space, and the above examples indicate how convergence in the flat norm is related to concepts of spectral convergence.

We recall that a sequence $\mu^{(k)}$ of Radon measures by definition converges weak* to a Radon measure μ if $\int \varphi d\mu^{(k)} \rightarrow \int \varphi d\mu$ for all continuous φ with compact support. In that case, in particular we have for each compact set K $|\mu^{(k)}|(K) \leq C(K)$.

One important property of the flat norm is that it metrizes weak* convergence of measures, in the following sense. Here and in the following, $\mathcal{M}(\mathbb{R}^n)$ denotes the space of Radon measures on \mathbb{R}^n .

Proposition 3.2. *Let μ_k be Radon measures supported in a compact set $K \subset \mathbb{R}^n$.*

- (i) *If $\mu_k \xrightarrow{*} \mu$ in $\mathcal{M}(\mathbb{R}^n)$, then $\|\mu_k - \mu\| \rightarrow 0$.*
- (ii) *If $\|\mu_k - \mu\| \rightarrow 0$ and the mass of the μ_k is uniformly bounded, then $\mu_k \xrightarrow{*} \mu$ in $\mathcal{M}(\mathbb{R}^n)$.*

Proof. We recall the proof for the convenience of the reader. The first assertion follows from the compactness of Lipschitz functions with respect to uniform convergence. Indeed we may assume that $\mu = 0$ and we have to show that $\|\mu_k\| \rightarrow 0$. Suppose otherwise. Then there exists a $\delta > 0$, a subsequence of μ_k (not relabelled) and a sequence of functions f_k such that $|f_k| \leq 1$, $\text{Lip } f_k \leq 1$, and $\int f_k d\mu_k \geq \delta$. For a further subsequence we have $f_k \rightarrow f$ uniformly in K . By weak* convergence the mass $\|\mu_k\|_{\mathcal{M}}$ of the measures μ_k is uniformly bounded. Thus

$$\limsup_{k \rightarrow \infty} \int f_k d\mu_k \leq \limsup_{k \rightarrow \infty} \left(\int f d\mu_k + \sup_K |f_k - f| \sup_k \|\mu_k\|_{\mathcal{M}} \right) = 0. \quad (3.3)$$

This contradiction proves assertion (i).

As regards (ii), we first observe that μ has bounded mass. Indeed for all Lipschitz functions f

$$\int f d\mu = \lim_{k \rightarrow \infty} \int f d\mu_k \leq \sup_K |f| \sup_k \|\mu_k\|_{\mathcal{M}}. \quad (3.4)$$

Thus we may suppose again that $\mu = 0$. Now let $f \in C(\mathbb{R}^n)$, $\epsilon > 0$. Then there exists a Lipschitz function g such that $\sup_K |f - g| < \epsilon$. Thus

$$\limsup_{k \rightarrow \infty} \left| \int f d\mu_k \right| \leq \limsup_{k \rightarrow \infty} \left| \int g d\mu_k \right| + \epsilon \sup_k \|\mu_k\|_{\mathcal{M}} \leq C\epsilon. \quad (3.5)$$

This proves assertion (ii) since $\epsilon > 0$ is arbitrary. \square

4. Variational Integrators

Let \mathcal{T}_h be a triangulation of \mathbb{R} of size h . Specifically, \mathcal{T}_h is a collection of ordered disjoint open intervals (t_i, t_{i+1}) whose closures cover the entire real line, and whose lengths are

less than or equal to h . Let X_h be the subspace of X consisting of continuous functions such that $u|_E \in P_1(E)$, $\forall E \in \mathcal{T}_h$. Here $P_k(E)$ denotes the set of polynomials over E of degree less than or equal to k . Define the discrete action functionals $I_h: X \times \mathcal{E} \rightarrow \mathbb{R}$ as

$$I_h(u, A) = \begin{cases} I(u, A), & u \in X_h, \\ +\infty, & \text{otherwise.} \end{cases} \quad (4.1)$$

The stationary points of I_h , or discrete solutions, are functions such that

$$\begin{aligned} I(u_h, A) &< \infty, & \delta I(u_h, \varphi_h, A) &= 0, \\ \forall A \in \mathcal{E}, \varphi_h &\in X_h, & \text{with } \varphi_h &= 0 \quad \text{on } \mathbb{R} \setminus A. \end{aligned} \quad (4.2)$$

Remark 4.1. In (4.2) it suffices to consider intervals (t_i, t_j) that are compatible with the triangulation \mathcal{T}_h . Indeed if (a, b) is a general interval and (t_i, t_j) is the maximal compatible subinterval, then the conditions $\varphi_h \in X_h$ and $\varphi = 0$ in $\mathbb{R} \setminus (a, b)$ imply that $\varphi = 0$ in (a, t_i) and (t_j, b) .

Let $E = (t_i, t_{i+1}) \in \mathcal{T}_h$ and $u_i = u_h(t_i)$. Then the discrete Lagrangian is

$$L_d(u_i, u_{i+1}) = I_h(u, E). \quad (4.3)$$

For piecewise linear approximations this gives

$$L_d(u_i, u_{i+1}) = \frac{m}{2} \frac{(u_{i+1} - u_i)^2}{t_{i+1} - t_i} - \int_{t_i}^{t_{i+1}} V \left(\frac{t_{i+1} - t}{t_{i+1} - t_i} u_i + \frac{t - t_i}{t_{i+1} - t_i} u_{i+1} \right) dt. \quad (4.4)$$

In terms of the discrete Lagrangian, the discrete Euler-Lagrange equations take the form

$$D_2 L_d(u_{i-1}, u_i) + D_1 L_d(u_i, u_{i+1}) = 0, \quad (4.5)$$

or for piecewise linear approximations,

$$\begin{aligned} m \left\{ \frac{u_{i+1} - u_i}{t_{i+1} - t_i} - \frac{u_i - u_{i-1}}{t_i - t_{i-1}} \right\} \\ + \int_{t_i}^{t_{i+1}} DV(u_h(t)) \frac{t_{i+1} - t}{t_{i+1} - t_i} dt + \int_{t_{i-1}}^{t_i} DV(u_h(t)) \frac{t - t_{i-1}}{t_i - t_{i-1}} dt = 0. \end{aligned} \quad (4.6)$$

Lemma 4.2. Let $u \in X_h$ be a stationary point of the discrete action functional I_h . Assume in addition that V is C^2 and that there is a constant $C > 0$ such that $|D^2 V| \leq C$. Let $a < b$ be such that $b - a < \pi/\omega_0$ with $\omega_0 = \sqrt{C/m}$. Then u minimizes $I_h(\cdot, (a, b))$ among all functions $v \in X_h$ with $v = u$ on $\mathbb{R} \setminus (a, b)$.

Proof. The proof of Lemma 2.1 applies since X_h is a subspace of X . Note that functions in X_h are continuous; hence we do not need to distinguish between left and right limits at a and b . \square

As a first step to understand the relation between I_h and I , we show that the spaces X_h approach X as $h \rightarrow 0$.

- Lemma 4.3.** (a) *The sequence of spaces X_h is dense in X , i.e., for each $u \in X$ there exist $v_h \in X_h$ with $v_h \rightarrow u$ in X .*
 (b) *Suppose that $V \in C(\mathbb{R}^n)$ and $V(s) \leq C(1 + |s|^2)$. If A is an open bounded interval and if $I(u, A) < \infty$, then the sequence v_h in (a) can be chosen such that in addition $v_h|_A \rightarrow u|_A$ in $H^1(A, \mathbb{R}^n)$.*

Proof. Let $\eta \in C_0^\infty(-1, 1)$ be a mollifier with $\eta \geq 0$, $\int \eta = 1$, and define $\eta_h(x) = h^{-1}\eta(x/h)$. Let $N_h w$ denote the nodal interpolation of a function w with respect to the triangulation \mathcal{T}_h . For $u \in X$ define $T_h u = N_h(\eta_h * u)$ and set $v_h = T_h u$. We need to show that for every $R > 0$ we have

$$\int_{-R}^R |v_h - u|^2 dt \rightarrow 0. \quad (4.7)$$

By standard interpolation estimates

$$\int_{-R}^R |N_h w - w|^2 dt \leq Ch^2 \int_{-R-h}^{R+h} |\dot{w}|^2 dt. \quad (4.8)$$

Combining this with standard estimates for convolutions, we get

$$\begin{aligned} \int_{-R}^R |T_h u - u|^2 dt &\leq C \int_{-R-2h}^{R+2h} |u|^2 dt, \\ \int_{-R}^R |T_h u - u|^2 dt &\leq Ch^2 \int_{-R-2h}^{R+2h} |\dot{u}|^2 dt. \end{aligned} \quad (4.9)$$

Now let $\epsilon > 0$ and write $u = u^{(1)} + u^{(2)}$ with $u^{(1)} \in H^1((-2R, 2R), \mathbb{R}^n)$ and $\int_{-2R}^{2R} |u^{(2)}|^2 dt \leq \epsilon$. Then

$$\limsup_{h \rightarrow 0} \int_{-R}^R |T_h u - u|^2 dt \leq C\epsilon, \quad (4.10)$$

and this proves the first assertion.

The proof of the second assertion is almost the same. The main additional difficulty is that u may jump at the ends of the interval $A = (a, b)$ (note that u is continuous in (a, b) by the Sobolev embedding theorem and the left limit $u(a)$ and the right limit $u(b)$ are well-defined and finite). To handle this difficulty we first define approximations of u that are continuous in the slightly large interval $A_h = (a - 2h, b + 2h)$. Set

$$u_h(t) = \begin{cases} u(t), & t \leq a - 2h, \\ u(a), & a - 2h < t \leq a, \\ u(t), & a < t < b, \\ u(b), & b \leq t < b + 2h, \\ u(t), & t \geq b + 2h. \end{cases} \quad (4.11)$$

Let $v_h = T_h u_h$. Then $u_h - u \rightarrow 0$ in $L^2(\mathbb{R}, \mathbb{R}^n)$ and $v_h - u = T_h(u_h - u) + (T_h u - u)$. Hence by the boundedness of T_h on L^2 (see (4.9)) and the proof of assertion (a) we have

$v_h \rightarrow u$ in X . To establish the convergence in $H^1(A, \mathbb{R}^n)$ we first recall the standard interpolation estimates

$$\begin{aligned} \int_a^b \left| \frac{d}{dt}(N_h w - w) \right|^2 &\leq \int_{a-h}^{b+h} \left| \frac{d}{dt} w \right|^2, \\ \int_a^b \left| \frac{d}{dt}(N_h w - w) \right|^2 &\leq Ch^2 \int_{a-h}^{b+h} \left| \frac{d^2}{dt^2} w \right|^2. \end{aligned} \quad (4.12)$$

Since $I(u, A) < \infty$, the map u is in $H^1(A, \mathbb{R}^n)$. Now decompose $u|_A = u^{(1)} + u^{(2)}$ such that $u^{(1)} \in H^2(A, \mathbb{R}^n)$ with $\dot{u}^{(1)}(a) = \dot{u}^{(1)}(b) = 0$ and $\|u^{(2)}\|_{H^1(A, \mathbb{R}^n)}^2 \leq \epsilon$. Combining the above interpolation estimates with standard estimates for convolutions such as

$$\begin{aligned} \int_{a-h}^{b+h} \left| \frac{d}{dt}(\eta_h * u - u) \right|^2 &\leq \int_{a-2h}^{b+2h} \left| \frac{d}{dt} u \right|^2, \\ \int_{a-h}^{b+h} \left| \frac{d}{dt}(\eta_h * u - u) \right|^2 &\leq Ch^2 \int_{a-2h}^{b+2h} \left| \frac{d^2}{dt^2} u \right|^2, \end{aligned} \quad (4.13)$$

we easily conclude that

$$\int_a^b \left| \frac{d}{dt}(v_h^{(1)} - u_h^{(1)}) \right|^2 \leq Ch^2, \quad \int_a^b \left| \frac{d}{dt}(v_h^{(2)} - u_h^{(2)}) \right|^2 \leq C\epsilon. \quad (4.14)$$

Taking first the limit $h \rightarrow 0$ and then $\epsilon \rightarrow 0$, we obtain assertion (b) since $u_h = u$ on (a, b) . \square

Lemma 4.4. *Let $V \in C(\mathbb{R}^n)$ with $V(s) \leq C(1 + |s|^2)$. Then $I(\cdot, (a, b))$ is lower semicontinuous in X .*

Proof. In view of the continuity and growth conditions on V , the map $u \rightarrow \int_a^b V(u) dt$ is continuous on $L^2((a, b), \mathbb{R}^n)$ and hence on X . Moreover the map $u \rightarrow \int_a^b \frac{m}{2} \dot{u}^2 dt$ is lower semicontinuous on $L^2((a, b), \mathbb{R}^n)$ since it is lower semicontinuous on the closed subspace $H^1((a, b), \mathbb{R}^n)$ (as a seminorm) and takes the value ∞ outside that subspace. \square

One key ingredient of our argument is that the functionals I_h are Γ -convergent to I . This is very closely related to convergence of the corresponding minimizers, and we will see that it can also be used to establish convergence of stationary points by restricting attention to sufficiently short intervals. For general information about Γ -convergence we refer to [3]. Here we only need the definition in the simplest case.

Definition 4.5. Let X be a metric space. We say that a sequence of functionals $I_h: X \rightarrow [-\infty, \infty]$ is Γ -convergent to I if

(i) (lower bound) Whenever $u_h \rightarrow u$ in X , then

$$\liminf_{h \rightarrow 0} I_h(u_h) \geq I(u); \quad (4.15)$$

- (ii) (upper bound/recovery sequence) for each $u \in X$, there exists a sequence $v_h \rightarrow u$ such that

$$\lim_{h \rightarrow 0} I_h(v_h) = I(u). \quad (4.16)$$

We write $\Gamma - \lim_{h \rightarrow 0} I_h = I$ to denote Γ -convergence.

Lemma 4.6. *Let $V \in C(\mathbb{R}^n)$ with $V(s) \leq C(1 + |s|^2)$. Then $\Gamma - \lim_{h \rightarrow 0} I_h(\cdot, (a, b)) = I(\cdot, (a, b))$ in X .*

Proof. Let $u_h \in X$ be a sequence converging to $u \in X$. From the fact that $I_h(\cdot, (a, b)) \geq I(\cdot, (a, b))$ and the lower semicontinuity of $I(\cdot, (a, b))$, it follows that $\liminf_h I_h(u_h, (a, b)) \geq \liminf_h I(u_h, (a, b)) = I(u, (a, b))$. Now let $u \in X$. If $I(u, A) = \infty$, there is nothing to show. If $I(u, A) < \infty$, then $u|_A \in H^1(A, \mathbb{R}^n)$. Hence by Lemma 4.3 there exist $u_h \in X_h$ such that $u_h|_A \rightarrow u|_A$ strongly in H^1 . Thus $I_h(u_h, A) \rightarrow I(u, A)$. \square

We now show that Γ -convergence implies convergence of stationary points. We first state an L^∞ version of the result and then make the connection with convergence of the Fourier transform in the flat norm.

Theorem 4.7. *Let I be an action functional. Assume that V is C^2 and that there is a constant $C > 0$ such that $|D^2 V| \leq C$. Let u_h be a sequence of stationary points of the corresponding discrete action integral I_h and suppose that u is bounded in $L^\infty(\mathbb{R}; \mathbb{R}^n)$. Then, for a subsequence,*

- (i) $u_h \xrightarrow{*} u$ in $W^{1,\infty}(\mathbb{R}, \mathbb{R}^n)$, and in particular $u_h \rightarrow u$ uniformly on compact subsets.
- (ii) u is a stationary point of I .

In general one cannot expect convergence of the full sequence. If, however, one knows that for some time T the pair $(u_h(T), \dot{u}_h(T))$ converges, then the full sequence u_h converges, by uniqueness for the limit problem (to see this, one makes use of the estimate (4.20)). A local version of the assertions of the theorem holds if we only assume a bound in L^∞_{loc} , which can be obtained in the usual way from bounds on the initial data and a discrete version of Gronwall's inequality. Global L^∞ bounds for the continuous solution follow from energy conservation if V converges to ∞ as $|u| \rightarrow \infty$. The same reasoning applies to the discrete solutions if a discrete energy is conserved. This can be achieved by also considering the discrete time points t_i as dependent variables (see [7], [10]), but the analysis of the resulting scheme is beyond the scope of this paper. For analytic V and under suitable assumptions on the limiting behaviour of the continuous solution at $\pm\infty$ and the discrete approximations, the convergence of discrete solutions was proved by Hairer and Lubich [5] through backward error analysis.

Corollary 4.8. *Let I be an action functional. Assume that V is C^2 and that there is a constant $C > 0$ such that $|D^2 V| \leq C$. Let u_h be a sequence of stationary points of the corresponding discrete action integral I_h , and let \hat{u}_h be the Fourier transform of u_h . Suppose that*

- (a) \hat{u}_h is a Radon measure of uniformly bounded mass.
 (b) No mass leaks to infinity in Fourier space, i.e.,

$$\lim_{R \rightarrow \infty} \sup_h \int_{|k| \geq R} |\hat{u}_h(k)| dk = 0. \quad (4.17)$$

Then, for a subsequence,

- (i) $u_h \xrightarrow{*} u$ in $W^{1,\infty}(\mathbb{R}; \mathbb{R}^n)$, and in particular $u_h \rightarrow u$ uniformly on compact subsets.
 (ii) u is a stationary point of I .
 (iii) $\hat{u}_h \rightarrow \hat{u}$ as measures in the flat norm.

To illustrate the assumptions on the Fourier transform we note that for stationary points of I , i.e., solutions of $\ddot{u} = -\nabla V(u)$, a sufficient condition for the Fourier transform to be a measure is that u approaches a constant or a periodic solution as $t \rightarrow \pm\infty$.

Proof of Theorem 4.7. By assumption we have for a subsequence (not relabelled) $u_h \xrightarrow{*} u$ in L^∞ . Since u_h satisfies the discrete Euler-Lagrange equations (4.6), we have

$$\begin{aligned} m \left| \frac{u_{i+1} - u_i}{t_{i+1} - t_i} - \frac{u_i - u_{i-1}}{t_i - t_{i-1}} \right| &\leq \left| \int_{t_i}^{t_{i+1}} DV(u_h(t)) \frac{t_{i+1} - t}{t_{i+1} - t_i} dt + \int_{t_{i-1}}^{t_i} DV(u_h(t)) \frac{t - t_{i-1}}{t_i - t_{i-1}} dt \right| \\ &\leq \left| \int_{t_i}^{t_{i+1}} DV(u_h(t)) \frac{t_{i+1} - t}{t_{i+1} - t_i} dt \right| + \left| \int_{t_{i-1}}^{t_i} DV(u_h(t)) \frac{t - t_{i-1}}{t_i - t_{i-1}} dt \right| \\ &\leq \int_{t_i}^{t_{i+1}} \left| DV(u_h(t)) \frac{t_{i+1} - t}{t_{i+1} - t_i} \right| dt + \int_{t_{i-1}}^{t_i} \left| DV(u_h(t)) \frac{t - t_{i-1}}{t_i - t_{i-1}} \right| dt \\ &\leq \int_{t_i}^{t_{i+1}} |DV(u_h(t))| dt + \int_{t_{i-1}}^{t_i} |DV(u_h(t))| dt = \int_{t_{i-1}}^{t_{i+1}} |DV(u_h(t))| dt. \end{aligned} \quad (4.18)$$

But, DV is continuous and $\|u_h\|_{L^\infty} \leq C$, and hence $\|DV(u_h)\|_{L^\infty} \leq C$ and

$$\left| \frac{u_{i+1} - u_i}{t_{i+1} - t_i} - \frac{u_i - u_{i-1}}{t_i - t_{i-1}} \right| \leq C |t_{i+1} - t_{i-1}|. \quad (4.19)$$

Iterating this bound, we obtain

$$|\dot{u}_h(a) - \dot{u}_h(b)| \leq C(|a - b| + 2h). \quad (4.20)$$

This inequality, together with the boundedness of u_h in L^∞ , implies that $\|\dot{u}_h\|_{L^\infty} \leq C$, and by the Arzela-Ascoli theorem we conclude that $u_h \rightarrow u$ uniformly on compact subsets and $u_h \xrightarrow{*} u$ in $W^{1,\infty}$. We claim that in addition $\|\ddot{u}\|_{L^\infty} \leq C$. Indeed consider again a standard mollifier $\eta_\delta(x) = \delta^{-1}\eta(x/\delta)$ as above and let $u_{h,\delta} = \eta_\delta * u_h$. It follows from (4.20) that

$$|\dot{u}_{h,\delta}(a) - \dot{u}_{h,\delta}(b)| \leq C(|a - b| + 2h + 2\delta). \quad (4.21)$$

We now take first the limit $h \rightarrow 0$ and then the limit $\delta \rightarrow 0$. Using the Lebesgue point theorem for \dot{u} we conclude that $|\dot{u}(a) - \dot{u}(b)| \leq C|a - b|$, which proves the claim.

To prove that u is a stationary point of I it suffices to show that u minimizes $I(\cdot, A)$ among functions with the same boundary values, for all sufficiently short intervals A . Fix $A = (a, b)$ with $b - a < \pi/\omega_0$, where $\omega_0 = \sqrt{C/m}$. We first note that, by Lemma 4.6, $\Gamma - \lim_{h \rightarrow 0} I_h(\cdot, (a, b)) = I(\cdot, (a, b))$ in X , and hence

$$\liminf_{h \rightarrow 0} I_h(u_h, (a, b)) \geq I(u, (a, b)). \quad (4.22)$$

Now consider a competitor $v \in X$ with $v \in H^1((a, b), \mathbb{R}^n)$ (here and in the following we write v instead of $v|_{(a,b)}$ to simplify the notation) with $v(a) = u(a)$ and $v(b) = u(b)$, where as usual $v(a)$ is the left-sided limit of v and $v(b)$ is the right-sided limit. We claim that

$$I(v, (a, b)) \geq I(u, (a, b)). \quad (4.23)$$

By Lemma 4.6 there exists a recovery sequence $v_h \in X_h$ with $v_h \rightarrow v$ in $H^1((a, b), \mathbb{R}^n)$ and

$$\lim_{h \rightarrow 0} I_h(v_h, (a, b)) = I(v, (a, b)). \quad (4.24)$$

If v_h and u_h agree and if the interval (a, b) is compatible with the triangulation \mathcal{T}_h (i.e., if a and b are endpoints of intervals in \mathcal{T}_h), we can use the minimizing property of u_h (see Lemma 4.2) to conclude. In general we can always find intervals $(a_h, b_h) \subset (a, b)$ that are compatible with \mathcal{T}_h such that $a_h \rightarrow a$ and $b_h \rightarrow b$. Since in view of the Sobolev embedding theorem $v_h \rightarrow v$ and $u_h \rightarrow u$ uniformly in (a, b) , we have $v_h(a_h) - u_h(a_h) \rightarrow v(a) - u(a) = 0$ and $v_h(b_h) - u_h(b_h) \rightarrow 0$. Hence there exist affine functions l_h , converging to zero in C^1 such that $v_h + l_h$ and u_h agree at a_h and b_h . Define $\tilde{v}_h \in X$ by $\tilde{v}_h = v_h + l_h$ in (a_h, b_h) , $\tilde{v}_h = u_h$ else. Now we can use the minimizing property of u_h to obtain

$$I_h(u_h, (a_h, b_h)) \leq I_h(\tilde{v}_h, (a_h, b_h)) = I_h(v_h + l_h, (a_h, b_h)). \quad (4.25)$$

Moreover (4.22) can be sharpened to

$$\liminf_{h \rightarrow 0} I_h(u_h, (a_h, b_h)) \geq I(u, (a, b)). \quad (4.26)$$

Indeed from strong L^2 convergence of u_h we deduce convergence of $\int_{a_h}^{b_h} V(u_h)$, and for the other term we first fix $a < a' < b' < b$. Observe that for sufficiently small h we have $\int_{a_h}^{b_h} |\dot{u}_h|^2 \geq \int_{a'}^{b'} |\dot{u}_h|^2$, use lower semicontinuity, and finally take the limit $a' \rightarrow a$, $b' \rightarrow b$. With the notation $A_h = (a_h, b_h)$ we finally get

$$\begin{aligned} I(u, A) &\leq \liminf_{h \rightarrow 0} I_h(u_h, A_h) \leq \liminf_{h \rightarrow 0} I_h(v_h + l_h, A_h) \\ &= \liminf_{h \rightarrow 0} I_h(v_h, A_h) = I(v, A), \end{aligned} \quad (4.27)$$

and this shows that u is minimizing. \square

Proof of Corollary 4.8. Since the mass of \hat{u}_h is bounded, u_h is bounded in L^∞ . Thus by Theorem 4.7 $u_h \xrightarrow{*} u$ in $W^{1,\infty}$ and u is a stationary point of I . Moreover, for a further subsequence, $\hat{u}_h \xrightarrow{*} \mu$ in \mathcal{M} . Thus $\mu = \hat{u}$. Finally, assumption (b) guarantees that $\|\hat{u}_h - \hat{u}\| \rightarrow 0$ (where $\|\cdot\|$ denotes the flat norm). Indeed, let $\varphi \in C_c^\infty(-1, 1)$, $\varphi = 1$ in $(-1/2, 1/2)$, and let $\varphi_R(k) = \varphi(k/R)$. Then $\varphi_R \hat{u}_h \xrightarrow{*} \varphi_R \hat{u}$ and, hence, $\|\varphi_R \hat{u}_h - \varphi_R \hat{u}\| \rightarrow 0$. But

$$\lim_{R \rightarrow \infty} \|(1 - \varphi_R) \hat{u}_h, (1 - \varphi_R) \hat{u}\| \leq 2 \lim_{R \rightarrow \infty} \sup_h \int_{|k| \geq R/2} |\hat{u}_h| dk = 0. \quad (4.28)$$

□

5. Numerical Integration

In practice the discrete Lagrangian L_d has to be computed by means of a numerical integration scheme, leading to a new discrete functional J_h . Our approach can easily be adapted to cover the convergence of stationary points of J_h to stationary points of I . The main elements of this extension are:

- (i) Gamma convergence: $\Gamma - \lim_{h \rightarrow 0} J_h = I$.
- (ii) Stationary points of J_h are minimizing on short intervals.
- (iii) A priori estimates for stationary points of J_h .

These properties hold for a large class of numerical quadrature schemes. For definiteness, here we restrict attention to the simple midpoint quadrature rule. Thus, if $(a, b) = (t_i, t_j)$ is an interval which is compatible with the triangulation \mathcal{T}_h , and if $u \in X_h$ (i.e., u is continuous and piecewise affine on \mathcal{T}_h), we set

$$\begin{aligned} J_h(u, (t_i, t_j)) &= \frac{m}{2} \sum_{l=i}^{j-1} (t_{l+1} - t_l) \left| \frac{u(t_{l+1}) - u(t_l)}{t_{l+1} - t_l} \right|^2 \\ &\quad + \sum_{l=i}^{j-1} (t_{l+1} - t_l) V \left(\frac{u(t_{l+1}) + u(t_l)}{2} \right). \end{aligned} \quad (5.1)$$

In order to study the convergence properties of J_h , it is convenient to extend the definition of J_h to intervals (a, b) that are not compatible with the triangulation \mathcal{T}_h . To this end, let (t_i, t_j) denote the largest subinterval of (a, b) that is compatible with the triangulation. Then we set

$$\begin{aligned} J_h(u, (a, b)) &= (t_i - a) \left[\frac{m}{2} \left| \frac{u(t_i) - u(t_{i-1})}{t_i - t_{i-1}} \right|^2 + V \left(\frac{u(t_i) + u(a)}{2} \right) \right] \\ &\quad + (b - t_j) \left[\frac{m}{2} \left| \frac{u(t_{j+1}) - u(t_j)}{t_{j+1} - t_j} \right|^2 + V \left(\frac{u(t_j) + u(b)}{2} \right) \right] \\ &\quad + J_h(u, (t_i, t_j)). \end{aligned} \quad (5.2)$$

Finally, if $u \notin X_h$, we set $J(u, (a, b)) = \infty$. As before, we say that u_h is a stationary point of J_h , or a discrete solution, if

$$\begin{aligned} J_h(u_h, A) &< \infty, & \delta J_h(u_h, \varphi_h, A) &= 0, \\ \forall A \in \mathcal{E}, \varphi_h \in X_h, & \text{ with } \varphi_h = 0 & \text{ on } \mathbb{R} \setminus A. \end{aligned} \quad (5.3)$$

Remark 4.1 still applies in the present setting, i.e., in (5.3) it suffices to consider intervals $A = (t_i, t_j)$ which are compatible with the triangulation \mathcal{T}_h . The discrete Euler-Lagrange equations again take the form

$$D_2 L_d(u_{i-1}, u_i) + D_1 L_d(u_i, u_{i+1}) = 0, \quad (5.4)$$

where the discrete Lagrangian is now given by

$$L_d(u_i, u_{i+1}) = \frac{m}{2} \frac{|u_{i+1} - u_i|^2}{t_{i+1} - t_i} - V\left(\frac{u_i + u_{i+1}}{2}\right)(t_{i+1} - t_i). \quad (5.5)$$

Again the convergence result can be stated in the L^∞ or the Fourier setting. For brevity, we only consider the latter.

Theorem 5.1. *Let I be an action functional. Assume that V is C^2 and that there is a constant $C > 0$ such that $|D^2 V| \leq C$. Let u_h be a sequence of stationary points of the discrete action integral J_h , and let \hat{u}_h be the Fourier transform of u_h . Suppose that*

- (a) \hat{u}_h is a Radon measure of uniformly bounded mass.
- (b) No mass leaks to infinity in Fourier space, i.e.,

$$\lim_{R \rightarrow \infty} \sup_h \int_{|k| \geq R} |\hat{u}_h(k)| dk = 0. \quad (5.6)$$

Then

- (i) $u_h \xrightarrow{*} u$ in $W^{1,\infty}(\mathbb{R}; \mathbb{R}^n)$.
- (ii) u is a stationary point of I .
- (iii) $\hat{u}_h \rightarrow \hat{u}$ as measures in the flat norm.

As mentioned above, the main new element in the proof of Theorem 5.1 is the following Γ -convergence result.

Lemma 5.2. *Under the assumptions of Theorem 5.1, we have*

$$\Gamma - \lim_{h \rightarrow 0} J_h(\cdot, (a, b)) = I(\cdot, (a, b)) \quad \text{in } X. \quad (5.7)$$

Proof. To separate the contributions of \dot{u} and $V(u)$, we define

$$\begin{aligned}
 J_{1,h}(u, (a, b)) &= \frac{m}{2} \sum_{l=i}^{j-1} (t_{l+1} - t_l) \left| \frac{u(t_{l+1}) - u(t_l)}{t_{l+1} - t_l} \right|^2 \\
 &\quad + \frac{m}{2} (t_i - a) \left| \frac{u(t_i) - u(t_{i-1})}{t_i - t_{i-1}} \right|^2 + \frac{m}{2} (b - t_j) \left| \frac{u(t_{j+1}) - u(t_j)}{t_{j+1} - t_j} \right|^2 \\
 &= \frac{m}{2} \int_a^b |\dot{u}|^2 dt, \\
 J_{2,h}(u, (a, b)) &= \sum_{l=i}^{j-1} (t_{l+1} - t_l) V\left(\frac{u(t_{l+1}) + u(t_l)}{2}\right) \\
 &\quad + (t_i - a) V\left(\frac{u(t_i) + u(a)}{2}\right) + (b - t_j) V\left(\frac{u(t_j) + u(b)}{2}\right).
 \end{aligned}$$

The upper bound for Γ -convergence follows directly from part (b) of Lemma 4.3. Indeed, if $u \in X = L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$ and $I(u, (a, b)) < \infty$, then there exist $v_h \in X_h$ with $v_h \rightarrow u$ in $H^1((a, b), \mathbb{R}^n)$. Therefore, $J_{1,h}(v_h, (a, b)) = \int_a^b |\dot{v}_h|^2 \rightarrow \int_a^b |\dot{u}|^2$. By the Sobolev embedding theorem we have that $v_h \rightarrow u$ uniformly, and from this we easily deduce that $J_{2,h}(v_h, (a, b)) \rightarrow \int_a^b V(u)$. This completes the proof of the upper bound.

For the lower bound we consider a sequence $u_h \rightarrow u$ in X . We may fix a subsequence such that $\liminf_{h \rightarrow 0} J_h(u_h, (a, b))$ is actually a limit. Note that for any interval (t_i, t_{i+1}) of the triangulation \mathcal{T}_h we have

$$\begin{aligned}
 \int_{t_i}^{t_{i+1}} u_h^2 dt &= \frac{1}{3} (t_{i+1} - t_i) (u_h^2(t_i) + u_h^2(t_{i+1}) + u_h(t_i)u_h(t_{i+1})) \\
 &\geq \frac{1}{6} (t_{i+1} - t_i) (u_h^2(t_i) + u_h^2(t_{i+1})).
 \end{aligned} \tag{5.8}$$

Thus

$$J_{2,h}(u_h, (a, b)) \leq C \int_{a-h}^{b+h} (1 + |u_h|^2) dt \leq C. \tag{5.9}$$

If $\lim_{h \rightarrow 0} J_h(u_h, (a, b)) = \infty$, there is nothing to show. Hence, we may suppose $\lim_{h \rightarrow 0} J_h(u_h, (a, b)) < \infty$ (along the subsequence chosen initially), and we thus have

$$\frac{m}{2} \int_a^b |\dot{u}_h|^2 dt = J_{1,h}(u_h, (a, b)) \leq C. \tag{5.10}$$

Therefore, $u_h \rightharpoonup u$ in $H^1((a, b), \mathbb{R}^n)$ and $\liminf_{h \rightarrow 0} J_{1,h}(u_h, (a, b)) \geq \int_a^b |\dot{u}|^2$. Moreover, by the Sobolev embedding theorem $u_h \rightarrow u$ uniformly, and thus $J_{2,h}(v_h, (a, b)) \rightarrow \int_a^b V(u)$. \square

Next we verify that stationary points of J_h are again minimizers on sufficiently short intervals.

Lemma 5.3. *Let u be a stationary point of the discrete functional J_h . Assume in addition that V is C^2 and that there is a constant $C > 0$ such that $|D^2V| \leq C$. Let $a < b$ be such that $b - a < 2/\omega_0$ with $\omega_0 = \sqrt{C/m}$. Then u minimizes $J_h(\cdot, (a, b))$ among all functions $v \in X_h$ with $u = v$ in $\mathbb{R} \setminus (a, b)$.*

Proof. It suffices to consider the case that $(a, b) = (t_i, t_j)$ is an interval compatible with the triangulation (see Remark 4.1). Using the discrete Euler-Lagrange equations (5.4), (5.5) and the Taylor expansion of V as in the proof of Lemma 2.1, we obtain the following for all $\varphi \in X_h$ that vanish at the endpoints a and b :

$$\begin{aligned} J_h(u + \varphi, (a, b)) - J_h(u, (a, b)) &\geq \frac{m}{2} \int_a^b |\dot{\varphi}|^2 - \frac{C}{2} \sum_{l=i}^{j-1} \left| \frac{\varphi(t_l) + \varphi(t_{l+1})}{2} \right|^2 \\ &\geq \frac{m}{2} \int_a^b |\dot{\varphi}|^2 - \frac{C}{2} (b - a) \sup |\varphi|^2 \\ &\geq \left(\frac{m}{2} - \frac{C(b-a)^2}{4} \right) \int_a^b |\dot{\varphi}|^2 \geq 0. \end{aligned} \quad \square$$

We finally prove Theorem 5.1.

Proof. The proof is very similar to that of Theorem 4.7. Again we have for a subsequence $u_h \xrightarrow{*} u$ in L^∞ and $\hat{u}_h \xrightarrow{*} \hat{u}$ in \mathcal{M} . The discrete Euler-Lagrange equations provide a $W^{1,\infty}$ estimate in complete analogy with (4.18). Indeed we have

$$\begin{aligned} \left| \frac{u_{i+1} - u_i}{t_{i+1} - t_i} - \frac{u_i - u_{i-1}}{t_i - t_{i-1}} \right| &\leq (t_{i+1} - t_i) \left| DV \left(\frac{u_{i+1} + u_i}{2} \right) \right| \\ &\quad + (t_i - t_{i-1}) \left| DV \left(\frac{u_i + u_{i-1}}{2} \right) \right|. \end{aligned} \quad (5.11)$$

Since DV is continuous and $\|u_h\|_{L^\infty} \leq C$, we get (4.19) again, i.e.,

$$\left| \frac{u_{i+1} - u_i}{t_{i+1} - t_i} - \frac{u_i - u_{i-1}}{t_i - t_{i-1}} \right| \leq C |t_{i+1} - t_{i-1}|. \quad (5.12)$$

Iterating the bound, we obtain as before (4.20) and deduce $u_h \xrightarrow{*} u$ in $W^{1,\infty}$. Now the proof can be finished exactly like the proof of Theorem 4.7, replacing I_h by J_h and using the Γ -convergence of J_h . \square

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References

- [1] Belytschko, T., and R. Mullen [1976], Mesh partitions of explicit–implicit time integrators. In K.-J. Bathe, J. T. Oden, and W. Wunderlich, editors, *Formulations and Computational Algorithms in Finite Element Analysis*, 673–690. MIT Press, Cambridge, Mass.
- [2] Belytschko, T. [1981], Partitioned and adaptive algorithms for explicit time integration. In W. Wunderlich, E. Stein, and K.-J. Bathe, editors, *Nonlinear Finite Element Analysis in Structural Mechanics*, 572–584. Springer-Verlag, New York.
- [3] DalMaso, G. [1993], *An introduction to Γ -convergence*. Birkhäuser, Boston-Basel-Berlin.
- [4] DeGiorgi, E., and T. Franzoni [1975], Su un tipo di convergenza variazionale, *Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur.* (8), **58**, 841–850.
- [5] Hairer, E., and C. Lubich [1997], The life-span of backward error analysis for numerical integrators, *Numerische Mathematik*, **76**, 441–462.
- [6] Hughes, T. J. R. [1987], *The Finite Element Method: Linear Static and Dynamic Finite Element Analysis*. Prentice-Hall, Englewood Cliffs, N.J.
- [7] Kane, C., J. E. Marsden, and M. Ortiz [1999], Symplectic energy-momentum integrators, *J. Math. Phys.*, **40**, 3353–3371.
- [8] Maggi, F., and M. Morini [2003], A Γ -convergence result for variational integrators of quadratic Lagrangians, Preprint 03-CNA-008, Carnegie Mellon University.
- [9] Marsden, J. E., G. W. Patrick, and S. Shkoller [1998], Multisymplectic geometry, variational integrators and nonlinear PDEs, *Commun. Math. Phys.*, **199**, 351–395.
- [10] Marsden, J. E. and M. West [2001], Discrete variational mechanics and variational integrators, *Acta Numerica*, **10**, 357–514.
- [11] Moser, J., and A. P. Veselov [1991], Discrete versions of some classical integrable systems and factorization of matrix polynomials, *Commun. Math. Phys.*, **139**, 217–243.
- [12] Reich, S. [1999], Backward error analysis for numerical integrators, *SIAM J. Num. Anal.*, **36**, 1549–1570.
- [13] Veselov, A. P. [1988], Integrable discrete-time systems and difference operators, *Funct. Anal. & Appl.*, **22**, 83–93.
- [14] Wendlandt, J. M., and J. E. Marsden [1997], Mechanical integrators derived from a discrete variational principle, *Physica D*, **106**, 223–246.