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by

Stefan Müller and Michael Ortiz

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ON THE Γ-CONVERGENCE OF DISCRETE DYNAMICS AND VARIATIONAL INTEGRATORS

STEFAN MÜLLER * AND MICHAEL ORTIZ †

Abstract. For a simple class of Lagrangians and variational integrators, derived by time discretization of the action functional, we supply conditions ensuring: i) The Γ-convergence of the discrete action sum to the action functional; ii) The weak* convergence of the discrete trajectories in $W^{1,\infty}(\mathbb{R})$ and uniform convergence on compact subsets; and iii) The convergence of the Fourier transform of the discrete trajectories as measures in the flat norm.

Key words. Discrete dynamics, Variational integrators, Gamma-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 [8], 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 [11] (see also [9]) showed that the discrete Euler-Lagrange equations generate symplectic maps. Wendlandt and Marsden [12] 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 [12] 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.* [7], it is possible to devise variational integrators which preserve the energy, momentum and symplectic structure, as shown by Kane *et al.* [5]. Extensions of the theory to partial differential equations based on multisymplectic geometry may be found in [7].

The convergence properties of variational integrators have been ascertained using conventional techniques, such as Gronwall's inequality [8]; or by backward error analysis [6, 10, 8]. In addition, time-stepping algorithms for linear structural dynamics have also been traditionally analyzed by *phase-error analysis* [1, 2, 4]. 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 in as much as it establishes the convergence of solutions in a global, instead of merely local, sense. In particular, it allows to compare infinite wave trains. The engineering literature on the subject 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

*Max Planck Institute for Mathematics in the Sciences, Inselstrasse 22, 04103 Leipzig, Germany
†Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 90025

of phase-error analysis to nonlinear systems appear to be in existence.

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 which appears not to have been pursued to date. In the work presented in this paper, we focus on a simple class of Lagrangians and variational integrators and supply conditions ensuring:

(i) The Γ-convergence of the discrete action sum to the action functional.

(ii) The weak* convergence of the discrete trajectories in $W^{1,\infty}(\mathbb{R})$ and uniform convergence on compact subsets.

iii) The convergence of the Fourier transform of the discrete trajectories as measures in the flat norm.

It bears emphasis that these notions of convergence are not local, as those derived from consistency and Gronwall's inequality, but apply to infinite wave trains. In particular, (iii) gives rigorous form to the traditional notions of phase-error analysis and spectral convergence, and extends them to nonlinear systems. While in this paper we focus on a simple class of Lagrangians in order to minimize technicalities, we would like to emphasize that the Γ−convergence framework is very flexible and should permit the analysis of much more general Lagrangians than considered here.

2. Formulation of the problem. Let $X = L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$, and let $\mathcal{E}$ be the collection of all open bounded intervals of $\mathbb{R}$. We recall that the spaces $L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$ 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 which $L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$ becomes a complete metric space. Let $m > 0$ and $V \in C(\mathbb{R}^n)$. The functional $I : X \times \mathcal{E} \to \mathbb{R}$ defined by

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

is the action of u over the open bounded interval A. The first variation of I is the functional $\delta I : H^1_{\text{loc}}(\mathbb{R}, \mathbb{R}^n) \times C_c^\infty(\mathbb{R}, \mathbb{R}^n) \times \mathcal{E} \to \mathbb{R}$ defined by

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

The stationary points of I are functions u such that

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

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 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 2.1. *For a general function $v \in X$ 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 $v_{|(a,b)} \in H^1\big((a, b), \mathbb{R}^n\big)$ and hence the one-sided limits $v(a)$ and $v(b)$ exist in view of the Sobolev embedding theorem.*

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

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

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

$$I(u + \varphi, (a, b)) - I(u, (a, b)) = \int_a^b \Big(\frac{m}{2}\dot\varphi^2(t) - V(u(t) + \varphi(t)) + V(u(t)) + DV(u(t)) \cdot \varphi(t) \Big)\, dt. \tag{2.5}$$

But by Taylor's theorem we have

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

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

$$|V(u + \varphi) - V(u) - DV(u)\varphi| \le \frac{C}{2}|\varphi|^2 \tag{2.7}$$

and

$$I(u+\varphi, (a, b))-I(u, (a, b)) \ge \int_a^b \Big(\frac{m}{2}\dot\varphi^2 - \frac{C}{2}|\varphi|^2 \Big)\, dt \ge \Big(\frac{m}{2}\frac{\pi^2}{(b-a)^2} - \frac{C}{2} \Big) \int_a^b |\varphi|^2\, dt, \tag{2.8}$$

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

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

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

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*

$$||\mu|| = \sup\{\int_{\mathbb{R}^n} f d\mu \,|\, f : \mathbb{R} \to \mathbb{R} \text{ Lipschitz}, \ \mathrm{Lip}\, f \le 1, \sup |f| \le 1\} \tag{3.1}$$

As a direct consequence of the definition one obtains

$$||\delta_a|| = 1, \qquad ||\delta_a - \delta_b|| = \min(|a - b|, 2) \tag{3.2}$$

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.

One important property of the flat norm is that it metrizes weak* convergence of measures, in the following sense.

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

i) If $\mu_k \overset{*}{\rightharpoonup} \mu$ in $\mathcal{M}(\mathbb{R}^n)$, then $||\mu_k - \mu|| \to 0$.

ii) If $||\mu_k - \mu|| \to 0$ and the mass of the μ_k is uniformly bounded, then $\mu_k \overset{*}{\rightharpoonup} \mu$ 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 $||\mu_k|| \to 0$. Suppose otherwise. Then there exists a $\delta > 0$, a subsequence of μ_k (not relabelled) and a sequence of functions f_k such that $|f_k| \leq 1$, $\mathrm{Lip} f_k \leq 1$ and $\int f_k d\mu_k \geq \delta$. For a further subsequence we have $f_k \to f$ uniformly in K. By weak* convergence the mass $||\mu_k||_{\mathcal{M}}$ of the measures μ_k is uniformly bounded. Thus

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

This contradiction proves assertion i).

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

$$\int f d\mu = \lim_{k\to\infty} \int f d\mu_k \leq \sup_K |f| \ \sup_k ||\mu_k||_{\mathcal{M}}. \tag{3.4}$$

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

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

This proves assertion ii) since $\epsilon > 0$ was arbitrary. □

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 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 or equal to k. Define the discrete action functionals $I_h : X \times \mathcal{E} \to \mathbb{R}$ as

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

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

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

REMARK 4.1. *In (4.2) it suffices to consider intervals (t_i, t_j) which 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

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

For piecewise linear approximations this gives

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

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

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

or, for piecewise linear approximations,

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

LEMMA 4.1. *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 $|D^2V| \le C$. Let $a < b$ be such that 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. □

LEMMA 4.2.

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 $v_h \to u$ in X.

b) Suppose that $V \in C(\mathbb{R}^n)$ and $V(s) \le C(1 + |s|^2)$. 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 $v_{h|A} \to u_{|A}$ in $H^1(A, \mathbb{R}^n)$.

Proof. Let $\eta \in C_0^\infty(-1, 1)$ be a mollifier with $\eta \ge 0$, $\int \eta = 1$, 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

$$\int_{-R}^{R} |v_h - u|^2\,dt \to 0 \tag{4.7}$$

By standard interpolation estimates

$$\int_{-R}^{R} |N_h w - w|^2\,dt \le Ch^2 \int_{-R-h}^{R+h} |\dot w|^2\,dt. \tag{4.8}$$

Combining this with standard estimates for convolutions we get

$$\int_{-R}^{R} |T_h u - u|^2\,dt \le C\int_{-R-2h}^{R+2h} |u|^2\,dt, \quad \int_{-R}^{R} |T_h u - u|^2\,dt \le Ch^2\int_{-R-2h}^{R+2h} |\dot u|^2\,dt. \tag{4.9}$$

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

$$\limsup_{h\to 0} \int_{-R}^{R} |T_h u - u|^2\,dt \le C\epsilon \tag{4.10}$$

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 which are continuous in the slightly large interval $A_h = (a - 2h, b + 2h)$.

Set

$$u_h(t) = \begin{cases} u(t), & t \le a - 2h \\ u(a), & a - 2h < t \le a \\ u(t) & a < t < b \\ u(b) & b \le t < b + 2h \\ u(t) & t \ge b + 2h \end{cases} \tag{4.11}$$

Let $v_h = T_h u_h$ Then $u_h - u \to 0$ in $L^2(\mathbb{R}, \mathbb{R}^n)$ and $v_n - u = T_h(u_h - u) + (T_h u - u)$. Hence by the boundedness of T_h on L^2 (see (4.9)) and the proof of assertion a) we have $v_h \to u$ in X. To establish the convergence in $H^1(A, \mathbb{R}^n)$ we first recall the standard interpolation estimates

$$\int_a^b |\frac{d}{dt}(N_h w - w)|^2 \le \int_{a-h}^{b+h} |\frac{d}{dt} w|^2, \quad \int_a^b |\frac{d}{dt}(N_h w - w)|^2 \le Ch^2 \int_{a-h}^{b+h} |\frac{d^2}{dt^2} w|^2. \tag{4.12}$$

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 $||u^{(2)}||^2_{H^1(A,\mathbb{R}^n)} \le \epsilon$. Combining the above interpolation estimates with standard estimates for convolutions such as

$$\int_{a-h}^{b+h} |\frac{d}{dt}(\eta_h * u - u)|^2 \le \int_{a-2h}^{b+2h} |\frac{d}{dt} u|^2, \quad \int_{a-h}^{b+h} |\frac{d}{dt}(\eta_h * u - u)|^2 \le Ch^2 \int_{a-2h}^{b+2h} |\frac{d^2}{dt^2} u|^2 \tag{4.13}$$

we easily conclude that

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

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

Lemma 4.3. *Let $V \in C(\mathbb{R}^n)$ with $V(s) \le C(1 + |s|^2)$. Then $I(\cdot, (a, b))$ is lower semicontinuous in X.*

Proof. In view of the continuity and growth conditions on V the map $u \to \int_a^b V(u)dt$ is continuous on $L^2((a, b), \mathbb{R}^n)$ and hence on X. Moreover the map $u \to \int_a^b \frac{m}{2} \dot{u}^2 dt$ is lower semicontinous 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. □

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

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

$$\liminf_{h \to 0} I_h(u_h) \ge I(u); \tag{4.15}$$

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

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

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

LEMMA 4.5. *Let* $V \in C(\mathbb{R}^n)$ *with* $V(s) \leq C(1+|s|^2)$. *Then* $\Gamma - \lim_{h\to 0} I_h\big(\cdot,(a,b)\big) = I\big(\cdot,(a,b)\big)$ *in* X.

Proof. Let $u_h \in X$ be a sequence converging to $u \in X$. From the fact that $I_h\big(\cdot,(a,b)\big) \geq I\big(\cdot,(a,b)\big)$ and the lower semicontinuity of $I\big(\cdot,(a,b)\big)$, it follows that $\liminf_h I_h\big(u_h,(a,b)\big) \geq \liminf_h I\big(u_h,(a,b)\big) = I\big(u,(a,b)\big)$. 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 4.2 there exist $u_h \in X_h$ such that $u_{h|A} \to u_{|A}$ strongly in H^1. Thus $I_h(u_h,A) \to I(u,A)$. ☐

THEOREM 4.6. *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 *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.,

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

Then

i) $u_h \overset{*}{\rightharpoonup} u$ *in* $L^\infty(\mathbb{R})$ *and* $W^{1,\infty}(\mathbb{R})$ *and* $u_h \to u$ *uniformly on compact subsets.*

ii) u *is a stationary point of* I.

iii) $\hat{u}_h \to \hat{u}$ *as measures in the flat norm.*

Proof. The sequence u_h is bounded in L^∞ since $\mathrm{mass}(\hat{u}_h) \equiv ||\hat{u}_h||_{\mathcal{M}}$ is bounded. Hence, there is a subsequence, relabelled u_h, such that

$$u_h \overset{*}{\rightharpoonup} u \quad \text{in } L^\infty. \tag{4.18}$$

At the same time,

$$\hat{u}_h \overset{*}{\rightharpoonup} \mu \quad \text{in } \mathcal{M}. \tag{4.19}$$

Hence, $\mu = \hat{u}$. But u_h is a stationary point of I_h and, consequently, it satisfies the discrete Euler-Lagrange equations (4.6), whence we have

$$\begin{aligned}
&m\left|\frac{u_{i+1}-u_i}{t_{i+1}-t_i} - \frac{u_i-u_{i-1}}{t_i-t_{i-1}}\right| \leq \\
&\left|\int_{t_i}^{t_{i+1}} DV\big(u_h(t)\big)\frac{t_{i+1}-t}{t_{i+1}-t_i}\,dt + \int_{t_{i-1}}^{t_i} DV\big(u_h(t)\big)\frac{t-t_{i-1}}{t_i-t_{i-1}}\,dt\right| \leq \\
&\left|\int_{t_i}^{t_{i+1}} DV\big(u_h(t)\big)\frac{t_{i+1}-t}{t_{i+1}-t_i}\,dt\right| + \left|\int_{t_{i-1}}^{t_i} DV\big(u_h(t)\big)\frac{t-t_{i-1}}{t_i-t_{i-1}}\,dt\right| \leq \\
&\int_{t_i}^{t_{i+1}} \left|DV\big(u_h(t)\big)\frac{t_{i+1}-t}{t_{i+1}-t_i}\right|dt + \int_{t_{i-1}}^{t_i} \left|DV\big(u_h(t)\big)\frac{t-t_{i-1}}{t_i-t_{i-1}}\,dt\right| \leq \\
&\int_{t_i}^{t_{i+1}} |DV\big(u_h(t)\big)|\,dt + \int_{t_{i-1}}^{t_i} |DV\big(u_h(t)\big)| = \int_{t_{i-1}}^{t_{i+1}} |DV\big(u_h(t)\big)|\,dt
\end{aligned} \tag{4.20}$$

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

$$\left|\frac{u_{i+1}-u_i}{t_{i+1}-t_i} - \frac{u_i-u_{i-1}}{t_i-t_{i-1}}\right| \leq C|t_{i+1}-t_{i-1}|. \tag{4.21}$$

Iterating this bound we obtain

$$|\dot{u}_h(a) - \dot{u}_h(b)| \le C(|a-b| + 2h). \tag{4.22}$$

This inequality, together with the boundedness of u_h in L^∞, implies that $||\dot{u_h}||_{L^\infty} \le C$, and by the Arzela-Ascoli theorem we conclude that $u_h \to u$ uniformly on compact subsets and $u_h \overset{*}{\rightharpoonup} u$ in $W^{1,\infty}$. We claim that in addition $||\ddot{u}||_{L^\infty} \le C$. 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 (4.22) that

$$|\dot{u}_{h,\delta}(a) - \dot{u}_{h,\delta}(b)| \le C(|a-b| + 2h + 2\delta). \tag{4.23}$$

We now take first the limit $h \to 0$ and then the limit $\delta \to 0$. Using the Lebesgue point theorem for $\dot{u}$ we conclude that $|\dot{u}(a) - \dot{u}(b)| \le C|a-b|$ 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 4.5, $\Gamma - \lim_{h\to 0} I_h\big(\cdot,(a,b)\big) = I\big(\cdot,(a,b)\big)$ in X, and hence

$$\liminf_{h\to 0} I_h\big(u_h,(a,b)\big) \ge I\big(u,(a,b)\big). \tag{4.24}$$

Now consider a competitor $v \in X$ with $v \in H^1\big((a,b),\mathbb{R}^n\big)$ (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

$$I\big(v,(a,b)\big) \ge I\big(u,(a,b)\big) \tag{4.25}$$

By Lemma 4.5 there exists a recovery sequence $v_h \in X_h$ with $v_h \to v$ in $H^1\big((a,b),\mathbb{R}^n\big)$ and

$$\lim_{h\to 0} I_h\big(v_h,(a,b)\big) = I\big(v,(a,b)\big) \tag{4.26}$$

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 4.1) to conclude. In general we can always find intervals $(a_h,b_h) \subset (a,b)$ which are compatible with $\mathcal{T}_h$ such that $a_h \to a$ and $b_h \to b$. Since in view of the Sobolev embedding theorem $v_h \to v$ and $u_h \to u$ uniformly in (a,b) we have $v_h(a_h) - u_h(a_h) \to v(a) - u(a) = 0$ and $v_h(b_h) - u_h(b_h) \to 0$. 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.

$$I_h\big(u_h,(a_h,b_h)\big) \le I_h\big(\tilde{v}_h,(a_h,b_h)\big) = I_h\big(v_h + l_h,(a_h,b_h)\big). \tag{4.27}$$

Moreover (4.24) can be sharpened to

$$\liminf_{h\to 0} I_h\big(u_h,(a_h,b_h)\big) \ge I\big((a,b),u\big). \tag{4.28}$$

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 $a' \to a$, $b' \to b$. With the notation $A_h = (a_h, b_h)$ we finally get

$$I(u,A) \leq \liminf_{h\to 0} I_h(u_h, A_h) \leq \liminf_{h\to 0} I_h(v_h + l_h, A_h) = \liminf_{h\to 0} I_h(v_h, A_h) = I(v, A) \tag{4.29}$$

and this shows that u is minimizing.

Finally, assumption (b) guarantees that $||\hat{u}_h - \hat{u}|| \to 0$ (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 $\varphi_R \hat{u}_h \stackrel{*}{\rightharpoonup} \varphi_R \hat{u}$ and, hence, $||\varphi_R \hat{u}_h - \varphi_R \hat{u}|| \to 0$. But

$$\lim_{R\to\infty} ||(1-\varphi_R)\hat{u}_h, (1-\varphi_R)\hat{u}|| \leq 2 \lim_{R\to\infty} \sup_h \int_{|k|\geq R/2} |\hat{u}_h| \, dk = 0. \tag{4.30}$$

□

5. Numerical integration. In practise 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: $\Gamma - \lim_{h\to 0} J_h = I$.

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 mid-point 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

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

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

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

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

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

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

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

where the discrete Lagrangian is now given by

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

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 $|D^2 V| \le C$. 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.,

$$\lim_{R\to\infty} \sup_h \int_{|k|\ge R} |\hat{u}_h(k)|\, dk = 0 \tag{5.6}$$

Then

i) $u_h \overset{*}{\rightharpoonup} u$ in $L^\infty(\mathbb{R})$ and $W^{1,\infty}(\mathbb{R})$ and $u_h \to u$ uniformly on compact subsets.

ii) u is a stationary point of I.

iii) $\hat{u}_h \to \hat{u}$ 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*

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

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

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

The upper bound for Γ-convergence follows directly from part (b) of Lemma 4.2. Indeed, if $u \in X = L^2_{\text{loc}}(\mathbb{R}, \mathbb{R}^n)$ and $I\big(u,(a,b)\big) < \infty$ then there exist $v_h \in X_h$ with $v_h \to u$ in $H^1\big((a,b), \mathbb{R}^n\big)$. Therefore, $J_{1,h}\big(v_h,(a,b)\big) = \int_a^b |\dot{v}_h|^2 \to \int_a^b |\dot{u}|^2$. By the

Sobolev embedding theorem we have that $v_h \to u$ uniformly, and from this we easily deduce that $J_{2,h}\big(v_h,(a,b)\big) \to \int_a^b V(u)$. This completes the proof of the upper bound.

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

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

Thus

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

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

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

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

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 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 for all $\varphi \in X_h$ which vanish at the endpoints a and b

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

☐

We finally prove Theorem 5.1.

Proof. The proof is very similar to that of Theorem 4.6. Again we have for a subsequence $u_h \overset{*}{\rightharpoonup} u$ in L^∞ and $\hat{u}_h \overset{*}{\rightharpoonup} \hat{u}$ in $\mathcal{M}$. The discrete Euler-Lagrange equations provide a $W^{1,\infty}$ estimate in complete analogy with (4.20). Indeed we have

$$\left|\frac{u_{i+1}-u_i}{t_{i+1}-t_i} - \frac{u_i-u_{i-1}}{t_i-t_{i-1}}\right| \le (t_{i+1}-t_i)\left|DV(\frac{u_{i+1}+u_i}{2})\right| + (t_i-t_{i-1})\left|DV(\frac{u_i+u_{i-1}}{2})\right|. \tag{5.11}$$

Since DV is continuous and $\|u_h\|_{L^\infty} \le C$ we get (4.21) again, i. e.,

$$\left|\frac{u_{i+1}-u_i}{t_{i+1}-t_i} - \frac{u_i-u_{i-1}}{t_i-t_{i-1}}\right| \le C|t_{i+1}-t_{i-1}|. \tag{5.12}$$

Iterating the bound we obtain as before (4.22) and deduce $u_h \overset{*}{\rightharpoonup} u$ in $W^{1,\infty}$. Now the proof can be finished exactly as the proof of Theorem 4.6, replacing I_h by J_h and using the Γ-convergence of J_h. □

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