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High-order variational time integrators for particle dynamics

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Abstract

The general family of Galerkin variational integrators are analyzed and a complete classification of such methods is proposed. This classification is based upon the type of basis function chosen to approximate the trajectories of material points and the numerical quadrature formula used in time. This approach leads to the definition of arbitrarily high order method in time. The proposed methodology is applied to the simulation of brownout phenomena occurring in helicopter take-off and landing.

1 Introduction

The definition and the analysis of high order geometric numerical integrators appear to be one of the most interesting challenge to deal with in the context of the simulation of mechanical systems, even in infinite dimensional cases. The variational integrators framework developed by Marsden and West [9] is the most general and elegant tool for the study of geometric integrators. Indeed, well known methods, like Störmer–Verlet [9], Newmark [8] and symplectic partitioned Runge–Kutta [6, 9], fit in this framework. This approach can be used also for the study of fairly new methods, like the *Galerkin variational integrators* [7, 13, 12, 15], that will be analyzed in this paper.

Some of the cited articles already contains partial results for some particular Galerkin variational integrators: in all these papers the space of polynomials of degree at most N is used to approximate the space of trajectories and different quadrature rules are employed (Gauss–Legendre quadrature with N nodes [9] or Gauss–Legendre–Lobatto quadrature with $N+1$ nodes [13, 12]). In particular in [12] the equivalence between some Galerkin variational integrators and a particular class of Runge–Kutta methods has been proved. This equivalence determines the convergence properties of these methods. In [7] a fairly general error analysis is developed for the case of polynomial of degree at most N with any quadrature rule of order at least $2N+1$.

This paper introduces a new theoretical framework for the study of well-posedness and error analysis of Galerkin variational integrators. At our knowledge this framework is the most general and complete available in the literature and it includes, as special cases, the results of the previously cited works.

In Section 2 the weak formulation of Euler–Lagrange equation is derived, recalling some useful concepts of functional analysis. Section 3 and Section 4 are devoted to the analysis of the continuous problem and its Galerkin approximation. In particular Section 4 contains the results about well posedness and convergence properties of the numerical method. In Section 5 we apply the obtained results to analyze the numerical method based on polynomial spaces and Gauss quadrature rule. Finally, in Section 6 numerical results assessing the theory are discussed.

2 Weak formulation of Euler-Lagrange equations

The most general formulation of governing equations for the motion of a mechanical system is the principle of least action, or Hamilton's principle, according to which every system is characterized by the Lagrangian function L and the motion between two different configurations at the times t_1 and t_2 is a path $t \mapsto \boldsymbol{u}(t)$ such that the action integral

$$S \coloneqq \int_{t_1}^{t_2} L(\boldsymbol{u}(t), \dot{\boldsymbol{u}}(t), t)\, dt \tag{1}$$

takes its stationary values. Under some regularity assumptions on the Lagrangian function, the calculus of variations ensures the equivalence between such principle and the Euler–Lagrange equations [1, Section 13]

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\boldsymbol{u}}} - \frac{\partial L}{\partial \boldsymbol{u}} = \boldsymbol{0}.$$

In general, the analysis of the mechanical problem can be hard and it depends on the properties of the Lagrangian function. In this paper we assume a Lagrangian of the canonical form

$$L(\boldsymbol{u}, \dot{\boldsymbol{u}}) = \frac{1}{2}\mu(\dot{\boldsymbol{u}}, \dot{\boldsymbol{u}}) - V(t, \boldsymbol{u}),$$

where μ is a given bilinear form and it can depend on time t, V is a given potential; moreover we also assume the presence of an external non-conservative force field $\boldsymbol{f}$ that depends on time t and position $\boldsymbol{u}$. From now on we assume that μ, V and $\boldsymbol{f}$ satisfy the following hypotheses:

- the form μ is uniformly bounded and elliptic in t, *i.e.* there exist two positive finite constants m and M such that

$$m\|\boldsymbol{u}\|^2 \leq \mu(\boldsymbol{u}, \boldsymbol{u}) \leq M\|\boldsymbol{u}\|^2, \qquad \forall \boldsymbol{u} \in \mathbb{R}^d;$$

- the potential V is differentiable with respect to the space coordinate, moreover the force field

$$\boldsymbol{F}_{\boldsymbol{u}}(t) \coloneqq \nabla V(t, \boldsymbol{u}) - \boldsymbol{f}(t, \boldsymbol{u})$$

is a uniformly Lipschitz continuous function in $\boldsymbol{u}$, *i.e.* there exists a finite positive constant K such that

$$\|\boldsymbol{F}_{\boldsymbol{u}_1}(t) - \boldsymbol{F}_{\boldsymbol{u}_2}(t)\| \leq K\|\boldsymbol{u}_1 - \boldsymbol{u}_2\|, \qquad \forall \boldsymbol{u}_1, \boldsymbol{u}_2 \in \mathbb{R}^d.$$

Thus the weak formulation of Euler–Lagrange equations with initial condition $(\boldsymbol{u}_0, \boldsymbol{p}_0)$ reads:

$$\int_0^h \mu(\dot{\boldsymbol{u}}, \dot{\boldsymbol{v}}) - \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{v}\, dt - (\boldsymbol{p}_h \cdot \boldsymbol{v}(h) - \boldsymbol{p}_0 \cdot \boldsymbol{v}(0)) = 0,$$

where $\boldsymbol{v}$ is a test function in some suitable function space, and $\boldsymbol{p}_0$, $\boldsymbol{p}_h$ are the linear momentum at times t_0 and t_h. In our formulation the initial condition is enforced in a weak sense hence $\boldsymbol{p}_h$ can be interpreted as the Lagrange's multiplier associated to the constraint $\boldsymbol{u}(0) = \boldsymbol{u}_0$.

In order to study the above mentioned problem and its approximation by means of a variational integrator a suitable functional setting should be provided. The problem is formulated in the Sobolev function space

$$X \coloneqq H^1(0,h) = \left\{ \boldsymbol{u} : [0,h] \to \mathbb{R}^n \;\middle|\; \boldsymbol{u} \in L^2(0,h) \text{ and } \dot{\boldsymbol{u}} \in L^2(0,h) \right\},$$

where $\dot{\boldsymbol{u}}$ denotes the weak derivative of $\boldsymbol{u}$ with respect to time. We equip this space with the less familiar norm defined by

$$\|\boldsymbol{u}\|_X^2 \coloneqq \int_0^h \|\dot{\boldsymbol{u}}\|^2\, dt + \frac{1}{h}\|\boldsymbol{u}(h)\|^2,$$

that is equivalent to the usual one for a Sobolev space. The equivalence is ensured by the Friedrichs' inequality [2, Section 6]

$$\|\boldsymbol{u}\|_0^2 \coloneqq \int_0^h \|\boldsymbol{u}\|^2\, dt \leq \frac{h^2}{z_0^2}\|\boldsymbol{u}\|_X^2,$$

where z_0 is the smaller positive solution of the equation $1 = z\tan z$, its approximated value is $z_0 \approx 0.86$. Using this norm it is easy to prove the continuity of the trace operator $\boldsymbol{u} \mapsto \boldsymbol{u}(h)$,

$$\|\boldsymbol{u}(h)\| \leq \sqrt{h}\|\boldsymbol{u}\|_X.$$

Remark 1 All the given inequalities are optimal, in the sense that always there exists a function $\boldsymbol{u}$ such that the equality is satisfied. For the Friedrichs' inequality this function is equal to $\boldsymbol{u} = \cos(z_0 t/h)$ whereas for the trace operator

it is enough to take the constant function. Moreover, these results are still valid using the equivalent norm

$$\|\boldsymbol{u}\|_X^2 \coloneqq \int_0^h \|\dot{\boldsymbol{u}}\|^2 \, dt + \frac{1}{h}\|\boldsymbol{u}(0)\|^2.$$

The equivalence is given by the invariance of the space X under the time inversion transformation $t \mapsto h - t$. □

Let $Q = \mathbb{R}^d$, then we can define the following bilinear forms

$$\begin{aligned} a &: X \times X \to \mathbb{R} & a(\boldsymbol{u}, \boldsymbol{v}) &\coloneqq \int_0^h \mu(\dot{\boldsymbol{u}}, \dot{\boldsymbol{v}}) \, dt, \\ b_1 &: X \times Q \to \mathbb{R} & b_1(\boldsymbol{u}, \boldsymbol{p}) &\coloneqq -\boldsymbol{u}(h) \cdot \boldsymbol{p}, \\ b_2 &: X \times Q \to \mathbb{R} & b_2(\boldsymbol{u}, \boldsymbol{p}) &\coloneqq -\boldsymbol{u}(0) \cdot \boldsymbol{p}, \end{aligned}$$

and recast the equations of motion in the following variational form: find $(\boldsymbol{u}, \boldsymbol{p}_h) \in X \times Q$ such that

$$\begin{cases} a(\boldsymbol{u}, \boldsymbol{v}) + b_1(\boldsymbol{v}, \boldsymbol{p}_h) = \displaystyle\int_0^h \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{v} \, dt + b_2(\boldsymbol{v}, \boldsymbol{p}_0), & \forall \boldsymbol{v} \in X, \\ b_2(\boldsymbol{u}, \boldsymbol{q}) + \boldsymbol{u}_0 \cdot \boldsymbol{q} = \boldsymbol{0}, & \forall \boldsymbol{q} \in Q. \end{cases} \tag{2}$$

In the next sections we are going to study the well-posedness of both Problem (2) and its Galerkin approximation. We also give a new proof of the convergence properties of such method; this proof is based on the abstract theory of saddle point problems [3, 11]. As in [3, 11] we denote with K_i the kernel of the operator associated with the form b_i $(i = 1, 2)$ and follows as

$$K_i \coloneqq \{\boldsymbol{u} \in X \mid b_i(\boldsymbol{u}, \boldsymbol{p}) = 0, \, \forall \boldsymbol{p} \in Q\}.$$

In some estimates we shall use the expression $A \lesssim B$ to say that there exists a constant C (that does not depend on A and B) such that $A \leq CB$.

3 Analysis of continuous problem

In this section we prove the existence and uniqueness of a solution of the Problem (2). These results are not really new since the equations of motion for a mechanical system are deeply understood. Nevertheless they are usually obtained using classical tools for ordinary differential equations, like the well known Picard–Lindelöf theorem; here we are going to study such equations starting from weak formulation. At our knowledge a complete analysis of the Lagrangian mechanics in this form has never been proposed. Moreover, our analysis provides the tools required to prove the well posedness and the convergence properties of the variational integrator that will be discussed in the next section. The main result of this section is the following theorem of existence and uniqueness for Problem (2).

Theorem 1 *For all initial condition* $(\boldsymbol{u}_0, \boldsymbol{p}_0)$ *and* h *such that*

$$\eta := \frac{3Kh^2}{mz_0^2} < 1,$$

there exists a unique solution $(\boldsymbol{u}, \boldsymbol{p}_h) \in X \times Q$ *of the Problem* (2)*. Moreover the solution map is Lipschitz continuous:*

$$\|\boldsymbol{u}^{(1)} - \boldsymbol{u}^{(2)}\|_X + \|\boldsymbol{p}_h^{(1)} - \boldsymbol{p}_h^{(2)}\| \lesssim \|\boldsymbol{u}_0^{(1)} - \boldsymbol{u}_0^{(2)}\| + \|\boldsymbol{p}_0^{(1)} - \boldsymbol{p}_0^{(2)}\|. \qquad \square$$

For the sake of clarity the proof of this theorem is preceded by two propositions where the hypotheses of the Theorem 3.1 in [11] are verified.

Proposition 1 *Given* $\boldsymbol{u} \in K_2$*, there exists* $\boldsymbol{v} \in K_1$ *such that:*

$$\frac{a(\boldsymbol{u}, \boldsymbol{v})}{\|\boldsymbol{v}\|_X} \geq \frac{m}{3}\|\boldsymbol{u}\|_X. \qquad \square$$

Proof Given $\boldsymbol{u} \in K_2$ ($\boldsymbol{u}(0) = \boldsymbol{0}$), then we take $\boldsymbol{v} = \boldsymbol{u} + \boldsymbol{\phi}$, where $\boldsymbol{\phi} \in X$ is the solution of the variational problem:

$$a(\boldsymbol{\phi}, \boldsymbol{\psi}) = \frac{m}{h}\boldsymbol{u}(h) \cdot \boldsymbol{\psi}(h), \quad \forall \boldsymbol{\psi} \in X.$$

Such problem admits a unique solution up to an additive constant which is chosen in order to satisfy the requirement $\boldsymbol{v} \in K_1$ ($\boldsymbol{v}(h) = \boldsymbol{0}$), so that

$$\boldsymbol{\phi}(h) = -\boldsymbol{u}(h).$$

Taking $\boldsymbol{\psi} = \boldsymbol{u}$, we have

$$a(\boldsymbol{u}, \boldsymbol{u} + \boldsymbol{\phi}) = a(\boldsymbol{u}, \boldsymbol{u}) + \frac{m}{h}\|\boldsymbol{u}(h)\|^2 \geq m\|\boldsymbol{u}\|_X^2. \tag{3}$$

On the other hand, taking $\boldsymbol{\psi} = \boldsymbol{\phi}$,

$$a(\boldsymbol{\phi}, \boldsymbol{\phi}) = \frac{m}{h}\boldsymbol{u}(h) \cdot \boldsymbol{\phi}(h).$$

From this identity, using the ellipticity of μ, we can bound the norm of $\boldsymbol{\phi}$

$$\|\boldsymbol{\phi}\|_X^2 \leq \frac{1}{m}a(\boldsymbol{\phi}, \boldsymbol{\phi}) + \frac{1}{h}\|\boldsymbol{\phi}(h)\|^2 \leq \frac{2}{h}\|\boldsymbol{u}(h)\|\|\boldsymbol{\phi}(h)\|,$$

and using the continuity of the trace operator $\boldsymbol{u} \mapsto \boldsymbol{u}(h)$, we obtain the estimate for the norm of $\boldsymbol{v}$:

$$\|\boldsymbol{v}\|_X = \|\boldsymbol{u} + \boldsymbol{\phi}\|_X \leq 3\|\boldsymbol{u}\|_X. \tag{4}$$

The proof is concluded combining (3) and (4). ■

Proposition 2 *The bilinear forms* b_i *satisfy the* $\inf - \sup$ *condition, in particular* $\beta_1 \geq h$*.* $\square$

PROOF For b_1 the proof is trivial, given $\boldsymbol{p}$ and chosen $\boldsymbol{v}$ to be constant and equal to $-\boldsymbol{p}$, then

$$\sup_{\boldsymbol{u}\in X} \frac{b_1(\boldsymbol{u},\boldsymbol{p})}{\|\boldsymbol{u}\|_X} \geq \frac{b_1(\boldsymbol{v},\boldsymbol{p})}{\|\boldsymbol{v}\|_X} \geq h\|\boldsymbol{p}\|.$$

The same holds for b_2 thanks to Remark 1. ∎

These propositions ensure the well-posedness of the linear part of the Problem (2) and we are going to exploit this partial result to give the proof of Theorem 1.

PROOF (PROOF OF THEOREM 1) Since we are dealing with a nonlinear problem, in order to prove the existence of a solution we define a sequence $\{\boldsymbol{u}^{(n)}\}_{n\in\mathbb{N}}$ obtained by iterating the solution map of a linearization of the original problem:

$$\begin{cases} a(\boldsymbol{u}^{(n)},\boldsymbol{v}) + b_1(\boldsymbol{v},\boldsymbol{p}_h^{(n)}) = \displaystyle\int_0^h \boldsymbol{F}_{\boldsymbol{u}^{(n-1)}}\cdot\boldsymbol{v}\,dt + b_2(\boldsymbol{v},\boldsymbol{p}_0), & \forall \boldsymbol{v}\in X,\\ b_2(\boldsymbol{u}^{(n)},\boldsymbol{q}) + \boldsymbol{u}_0\cdot\boldsymbol{q} = \boldsymbol{0}, & \forall \boldsymbol{q}\in Q. \end{cases}$$

Taking the difference between two subsequent iterations we obtain the problem:

$$\begin{cases} a(\boldsymbol{u}^{(n+1)}-\boldsymbol{u}^{(n)},\boldsymbol{v}) + b_1(\boldsymbol{v},\boldsymbol{p}_h^{(n+1)}-\boldsymbol{p}_h^{(n)}) = \\ \qquad = \displaystyle\int_0^h (\boldsymbol{F}_{\boldsymbol{u}^{(n)}} - \boldsymbol{F}_{\boldsymbol{u}^{(n-1)}})\cdot\boldsymbol{v}\,dt, & \forall \boldsymbol{v}\in X,\\ b_2(\boldsymbol{u}^{(n+1)}-\boldsymbol{u}^{(n)},\boldsymbol{q}) = \boldsymbol{0}, & \forall \boldsymbol{q}\in Q. \end{cases} \tag{5}$$

So, starting from $\boldsymbol{u}^{(0)}$ and $\boldsymbol{u}^{(1)}$ (for example taking the constant functions equal to $\boldsymbol{u}_0$), if the Problem (5) is well-posed, then it uniquely defines the sequence $\{\boldsymbol{u}^{(n)}\}_{n\in\mathbb{N}}$. Clearly all the bilinear forms are trivially continuous and all the other hypotheses of Theorem 3.1 in [11] are satisfied according to the results of Proposition 1 and Proposition 2. Then the Problem (5) admits a unique solution, moreover the following estimate holds:

$$\|\boldsymbol{u}^{(n+1)}-\boldsymbol{u}^{(n)}\|_X \leq \frac{3}{m}\|\boldsymbol{F}_{\boldsymbol{u}^{(n)}} - \boldsymbol{F}_{\boldsymbol{u}^{(n-1)}}\|_{X'}.$$

Now we should give an estimate of the right-hand side using the fact that the gradient of the potential V is a uniformly Lipschitz continuous function:

$$\left|\int_0^h (\boldsymbol{F}_{\boldsymbol{u}^{(n)}} - \boldsymbol{F}_{\boldsymbol{u}^{(n-1)}})\cdot\boldsymbol{v}\,dt\right| \leq K\|\boldsymbol{u}^{(n)}-\boldsymbol{u}^{(n-1)}\|_0\|\boldsymbol{v}\|_0,$$

using the Friedrichs' inequality we get

$$\|\boldsymbol{u}^{(n+1)}-\boldsymbol{u}^{(n)}\|_X \leq \frac{3Kh^2}{mz_0^2}\|\boldsymbol{u}^{(n)}-\boldsymbol{u}^{(n-1)}\|_X,$$

where we recognize the parameter η; if $\eta < 1$ then the solution map is contractive and in particular the sequence $\{\boldsymbol{u}^{(n)}\}_{n\in\mathbb{N}}$ is a Cauchy sequence. From the estimate for the second component of the solution

$$h\|\boldsymbol{p}_h^{(n+1)} - \boldsymbol{p}_h^{(n)}\| \leq \left(1 + \frac{3M}{m}\right) \|\boldsymbol{F}_{\boldsymbol{u}^{(n)}} - \boldsymbol{F}_{\boldsymbol{u}^{(n-1)}}\|_{X'},$$

we can state that also the sequence $\{\boldsymbol{p}_h^{(n)}\}_{n\in\mathbb{N}}$ is a Cauchy sequence. Hence both sequences converge to a limit $(\boldsymbol{u}, \boldsymbol{p}_h)$ in $X \times Q$ and by continuity of the terms of Problem (2) it follows that such limit is a solution.
In order to prove the continuity of the solution map, let us consider two different initial data $(\boldsymbol{u}_0^{(1)}, \boldsymbol{p}_0^{(1)})$ and $(\boldsymbol{u}_0^{(2)}, \boldsymbol{p}_0^{(2)})$. We have just proved that for both there exists at least one solution $(\boldsymbol{u}^{(i)}, \boldsymbol{p}_h^{(i)})$ of Problem (2), then taking the difference we obtain the problem:

$$\begin{cases} a(\boldsymbol{u}^{(1)} - \boldsymbol{u}^{(2)}, \boldsymbol{v}) + b_1(\boldsymbol{v}, \boldsymbol{p}_h^{(1)} - \boldsymbol{p}_h^{(2)}) = \\ \qquad = \displaystyle\int_0^h (\boldsymbol{F}_{\boldsymbol{u}^{(1)}} - \boldsymbol{F}_{\boldsymbol{u}^{(2)}}) \cdot \boldsymbol{v}\, dt + b_2(\boldsymbol{v}, \boldsymbol{p}_0^{(1)} - \boldsymbol{p}_0^{(2)}), & \forall \boldsymbol{v} \in X, \\ b_2(\boldsymbol{u}^{(1)} - \boldsymbol{u}^{(2)}, \boldsymbol{q}) + (\boldsymbol{u}_0^{(1)} - \boldsymbol{u}_0^{(2)}) \cdot \boldsymbol{q} = 0, & \forall \boldsymbol{q} \in Q. \end{cases}$$

From these equation, using the stability estimates of Theorem 3.1 in [11] the continuity of solution map is proved, under the same condition $\eta < 1$. The uniqueness easily follow from the continuity estimates. ∎

4 Analysis of Galerkin variational integrator

The aim of this section is to introduce a very general theory that can be used to develop a taxonomic scheme of the Galerkin variational integrators. For the sake of clarity we start from an informal introduction to the variational integrators. The reader is referred to [9] for the technical details.

The definition of variational integrators relies on the same principle of the continuous problem: each numerical integrator is characterized by the discrete Lagrangian function L_d. Given a discrete set of increasing times $t_0, t_1, \ldots, t_N$, the motion between two configurations $\boldsymbol{u}_0$ and $\boldsymbol{u}_N$ is the map $t_i \mapsto \boldsymbol{u}_i$ such that the discrete action given by

$$\sum_{i=0}^{N-1} L_d(\boldsymbol{u}_i, \boldsymbol{u}_{i+1}) \tag{6}$$

takes its stationary values. Then by the Fermat's theorem on the stationary points the discrete Euler-Lagrange equations read [9, Section 1.3.1]

$$D_2 L_d(\boldsymbol{u}_{i-1}, \boldsymbol{u}_i) + D_1 L_d(\boldsymbol{u}_i, \boldsymbol{u}_{i+1}) = \boldsymbol{0}, \qquad \forall i = 1, \ldots, N-1,$$

where D_i are the partial derivative operator with respect to the i-th argument. Comparing Equation (1) and Equation (6) we can see that the discrete Lagrangian

$L_d(\boldsymbol{u}_i, \boldsymbol{u}_{i+1})$ represents an approximation of the action integral

$$\int_{t_i}^{t_{i+1}} L(\boldsymbol{u}(t), \dot{\boldsymbol{u}}(t), t)\, dt,$$

and the obtained variational integrators is, in some sense, as good as this approximation. Thus the aim is to find a good trade-off between the complexity and the error in the evaluation of action.

The Galerkin method can be used for the definition and the analysis of arbitrarily high order numerical method for differential problems; the application of this technique in the context of variational integrators define the class of Galerkin variational integrators. Each Galerkin method is characterized by two elements:

- a finite dimensional space X_N of functions used for approximating the trajectory $t \mapsto \boldsymbol{u}(t)$. The space of polynomials of degree at most N is the most common choice, but other choices can be useful in some particular case, like the Fourier system in the case of periodic orbits. For the sake of simplicity we consider the problem for a d-dimensional mechanical system on the time interval $[0, h]$. The set of functions $\{\phi_i\}_{i=0}^{N} \subset C^1([0, h])$ span the space X_N, then each element $\boldsymbol{u} \in X_N$ can be written as

$$\boldsymbol{u}(t) = \sum_{i=0}^{N} \boldsymbol{u}^{(i)} \phi_i(t), \qquad \boldsymbol{u}^{(0)}, \ldots, \boldsymbol{u}^{(N)} \in \mathbb{R}^d.$$

- a quadrature rule used to evaluate the action integral. Without loss of generality we can assume that this rule is defined by a discrete set of $M+1$ quadrature points $\{t_k\}$ and positive weights $\{w_k\}$:

$$\int_{t_i}^{t_{i+1}} f(t)\, dt \approx \sum_{k=0}^{M} f(t_k) w_k.$$

  Again, the most common choices are the Gauss and Gauss–Lobatto quadrature rules, but it is not strictly required to adopt one of these two rules.

Given a path $\boldsymbol{u}_N \in X_N$, the discrete action functional is defined as

$$\mathcal{S}_N(\boldsymbol{u}_N) \coloneqq \sum_{k=0}^{M} L(\boldsymbol{u}_N|_k, \dot{\boldsymbol{u}}_N|_k, t_k) w_k,$$

then the discrete Lagrangian L_d reads

$$L_d(\boldsymbol{u}_0, \boldsymbol{u}_h) \coloneqq \inf\{\mathcal{S}_N(\boldsymbol{u}_N) \mid \boldsymbol{u}_N \in X_N \wedge \boldsymbol{u}_N(0) = \boldsymbol{u}_0 \wedge \boldsymbol{u}_N(h) = \boldsymbol{u}_h\}. \tag{7}$$

The solution of this variational problem is equivalent to the application of the GNI (Galerkin with Numerical Integration) method to the Problem (2), thus

the formulation of a Galerkin variational integrator becomes: find $(\boldsymbol{u}_N, \boldsymbol{p}_{h,N}) \in X_N \times Q$ such that

$$\begin{cases} a_N(\boldsymbol{u}_N, \boldsymbol{v}_N) + b_1(\boldsymbol{v}_N, \boldsymbol{p}_{h,N}) = \displaystyle\sum_{k=0}^{M} (\boldsymbol{F}_{\boldsymbol{u}_N} \cdot \boldsymbol{v}_N)|_k w_k + b_2(\boldsymbol{v}_N, \boldsymbol{p}_0), & \forall \boldsymbol{v}_N \in X_N, \\ b_2(\boldsymbol{u}_N, \boldsymbol{q}) + \boldsymbol{u}_0 \cdot \boldsymbol{q} = 0, & \forall \boldsymbol{q} \in Q, \end{cases} \tag{8}$$

where b_1 and b_2 are the bilinear forms already defined in Section 2 and $a_N : X_N \times X_N \to \mathbb{R}$ is defined by:

$$a_N(\boldsymbol{u}_N, \boldsymbol{v}_N) \coloneqq \sum_{k=0}^{M} \mu(\dot{\boldsymbol{u}}_N(t_k), \dot{\boldsymbol{v}}_N(t_k)) w_k.$$

To investigate the well-posedness in the discrete Problem (8) the same results exposed in the previous section for the continuous problem are exploited. For this reason we introduce two seminorms, the discrete counterpart of L^2 and H^1 norms:

$$|\boldsymbol{u}_N|_{0,N}^2 \coloneqq \sum_{k=0}^{M} \|\boldsymbol{u}_N(t_k)\|^2 w_k, \qquad \|\boldsymbol{u}_N\|_{X_N}^2 \coloneqq |\dot{\boldsymbol{u}}_N|_{0,N}^2 + \frac{1}{h}\|\boldsymbol{u}(h)\|^2.$$

In particular, if the following hypotheses are satisfied:

1. the subspace of constant functions is contained in X_N;
2. $\|\cdot\|_{X_N}$ defines a norm of the space X_N;

then Proposition 1 and Proposition 2 are still valid if we replace the bilinear form a with a_N and the norm $\|\cdot\|_X$ with $\|\cdot\|_{X_N}$. The first hypothesis does not represent a limitation since it is satisfied for all the finite dimensional spaces of practical relevance. The second hypothesis is harder to prove and it represents a compatibility condition between the space X_N and the quadrature rule. This hypothesis is not only a technical requirement for proving the well-posedness of Equations (8); the next lemma clarifies its physical meaning and gives a very important criterion for proving its validity.

Lemma 1 *If the subspace of constant functions is contained in X_N then the problem:*

$$\begin{cases} a_N(\boldsymbol{u}_N, \boldsymbol{v}_N) + b_1(\boldsymbol{v}_N, \boldsymbol{p}_{h,N}) = b_2(\boldsymbol{v}_N, \boldsymbol{p}_0), & \forall \boldsymbol{v}_N \in X_N, \\ b_2(\boldsymbol{u}_N, \boldsymbol{q}) + \boldsymbol{u}_0 \cdot \boldsymbol{q} = 0, & \forall \boldsymbol{q} \in Q. \end{cases} \tag{9}$$

admits a unique solution for all initial conditions $(\boldsymbol{u}_0, \boldsymbol{p}_0)$ if and only if $\|\cdot\|_{X_N}$ is a norm on the space X_N. □

Proof If $\|\cdot\|_{X_N}$ is a norm on the space X_N then the hypotheses of Theorem 3.1 in [11] are satisfied and Problem (9) admits a unique solution. To prove that

uniqueness implies that $\|\cdot\|_{X_N}$ is a norm we proceed by *reductio ad absurdum*. Assumed that the free system problem admits an unique solution and $\|\cdot\|_{X_N}$ is only a seminorm then there exists $\boldsymbol{w}_N \in X_N$ not equal to $\mathbf{0}$ such that $\|\boldsymbol{w}_N\|_{X_N} = 0$, that means:

$$\boldsymbol{w}_N(h) = \mathbf{0} \quad \text{and} \quad \dot{\boldsymbol{w}}_N(t_k) = \mathbf{0} \text{ for all } k = 0, \dots, M.$$

Now choose $\boldsymbol{v}_N = \boldsymbol{w}_N$ in the first equation of (9), thus

$$b_2(\boldsymbol{w}_N, \boldsymbol{p}_0) = \mathbf{0}, \qquad \forall \boldsymbol{p}_0 \in Q. \tag{10}$$

Now we have two alternatives:

- if $\boldsymbol{w}_N(0) = 0$ then Equation (10) is always true and if Problem (9) admits a solution $\boldsymbol{u}_N$ then $\boldsymbol{u}_N + \alpha \boldsymbol{w}_N$ is also a solution for any $\alpha \in \mathbb{R}$;
- if $\boldsymbol{w}_N(0) \neq 0$ then Equation (10) is never verified and the Problem (9) has no solutions.

This leads to the absurdum. ∎

In order to prove the well-posedness of the Problem (8) it is necessary to assume the validity of the Friedrichs' inequality in the space X_N, that reads

$$|\boldsymbol{u}_N|_{0,N} \leq C_N \frac{h}{z_0} \|\boldsymbol{u}_N\|_{X_N}, \quad \forall \boldsymbol{u}_N \in X_N, \tag{11}$$

where C_N is a positive constant that depends on the definition of space X_N, but not on h (by a scaling argument). Since X_N is finite dimension space then the Bolzano–Weierstrass theorem ensures the existence and the finiteness of such constant C_N, but its value could be not uniformly bounded with respect to N. In such case the next theorem states that in order to ensure the well-posedness of Problem (8) it is necessary to choose very small value for the time step h.

Theorem 2 *For all initial condition $(\boldsymbol{u}_0, \boldsymbol{p}_0)$ and h such that*

$$\eta = \frac{3Kh^2}{mz_0^2} < \frac{1}{C_N^2},$$

there exists a unique solution $(\boldsymbol{u}_N, \boldsymbol{p}_{h,N}) \in X_N \times Q$ of Problem (8). Moreover the solution map is Lipschitz continuous:

$$\|\boldsymbol{u}_N^{(1)} - \boldsymbol{u}_N^{(2)}\|_{X_N} + \|\boldsymbol{p}_{h,N}^{(1)} - \boldsymbol{p}_{h,N}^{(2)}\| \lesssim \|\boldsymbol{u}_0^{(1)} - \boldsymbol{u}_0^{(2)}\| + \|\boldsymbol{p}_0^{(1)} - \boldsymbol{p}_0^{(2)}\|. \qquad \square$$

Proof The proof follows exactly the same steps of the proof of Theorem 1. ∎

We now turn our attention to the the approximation property of the Galerkin variational integrators in the time interval $(0, h)$, deriving an estimate of the error $\|\boldsymbol{u} - \boldsymbol{u}_N\|_X$, where $\boldsymbol{u}$ and $\boldsymbol{u}_N$ are the solution of Problems (2) and (8)

respectively. The equivalence of all norms defined on a finite dimension vector space holds to the existence of $\Lambda_N \geq \lambda_N > 0$ such that

$$\lambda_N \|\boldsymbol{u}_N\|_X \leq \|\boldsymbol{u}_N\|_{X_N} \leq \Lambda_N \|\boldsymbol{u}_N\|_X, \quad \forall \boldsymbol{u}_N \in X_N. \tag{12}$$

Thanks to this equivalence we can compare the norm in the discrete and continuous settings and we can prove the following theorem following theorem, that be considered as an extension to the Galerkin variational integrators of the Strang's lemma [3, Theorem 2.2].

Theorem 3 *For any initial data $\boldsymbol{u}_0, \boldsymbol{p}_0$ and small enough h, the solutions $\boldsymbol{u}$ and $\boldsymbol{u}_N$ of Problems* (2) *and* (8) *satisfy the following estimate:*

$$(1-\Lambda_N C_N^2 \eta)\|\boldsymbol{u}-\boldsymbol{u}_N\|_X \lesssim \inf_{\boldsymbol{v}_N \in X_N} \left[\|\boldsymbol{u}-\boldsymbol{v}_N\|_X + \sup_{\boldsymbol{z}_N \in K_{1,N}} \frac{(a-a_N)(\boldsymbol{v}_N, \boldsymbol{z}_N)}{\|z_N\|_X} \right] + \\ + \sup_{\boldsymbol{z}_N \in K_{1,N}} \frac{1}{\|z_N\|_X} \left(\sum_{k=0}^{M} \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{z}_N|_k w_k - \int_0^h \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{z}_N \, dt \right).$$

In particular if both Λ_N and λ_N are uniformly bounded with respect to N then the constants appearing in this estimate does not depend on N. □

In this estimate we have three terms that bound the error $\|\boldsymbol{u}-\boldsymbol{u}_N\|_X$: the first one represents the *approximation error* associated to the definition of discrete space X_N, known as *approximation error*, the other two are related to the quadrature rule and they represent the *consistency error*. In order to balance the two components of the error the space X_N and the quadrature have to be chosen in a proper way.

Proof Using the equivalence (12) and Theorem 2.2 of [3] we deduce the following estimate: there exists $A_N > 0$ such that for all $\boldsymbol{v}_N \in X_N$

$$\|\boldsymbol{u}-\boldsymbol{u}_N\|_X \leq A_N \|\boldsymbol{u}-\boldsymbol{v}_N\|_X + \frac{3}{m} \sup_{\boldsymbol{z}_N \in K_{1,N}} \frac{(a-a_N)(\boldsymbol{v}_N, \boldsymbol{z}_N)}{\|z_N\|_{X_N}} + \\ + \frac{3}{m} \sup_{\boldsymbol{z}_N \in K_{1,N}} \frac{1}{\|z_N\|_{X_N}} \left(\sum_{k=0}^{M} \boldsymbol{F}_{\boldsymbol{u}_N} \cdot \boldsymbol{z}_N|_k w_k - \int_0^h \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{z}_N \, dt \right),$$

where the last term can be rewritten as

$$\sum_{k=0}^{M} (\boldsymbol{F}_{\boldsymbol{u}_N} - \boldsymbol{F}_{\boldsymbol{u}}) \cdot \boldsymbol{z}_N|_k w_k + \sum_{k=0}^{M} \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{z}_N|_k w_k - \int_0^h \boldsymbol{F}_{\boldsymbol{u}} \cdot \boldsymbol{z}_N \, dt.$$

Since the force field $\boldsymbol{F}_{\boldsymbol{u}}$ is assumed to be uniformly Lipschitz continuous, then

$$\sum_{k=0}^{M} (\boldsymbol{F}_{\boldsymbol{u}_N} - \boldsymbol{F}_{\boldsymbol{u}}) \cdot \boldsymbol{z}_N|_k w_k \leq C_N^2 \frac{Kh^2}{z_0^2} \|\boldsymbol{u}-\boldsymbol{u}_N\|_{X_N} \|z_N\|_{X_N}.$$

In order to conclude the proof is enough to use again the equivalence (12). ■

A second result about the approximation properties of the Galerkin variational integrators deals with the order of the discrete Hamiltonian map

$$(\boldsymbol{u}_0, \boldsymbol{p}_0) \mapsto (\boldsymbol{u}_{h,N}, \boldsymbol{p}_{h,N}), \quad \text{where } \boldsymbol{u}_{h,N} = \boldsymbol{u}_N(h).$$

This result is based on the general theory of the variational integrators exposed in [9] and in particular it is a corollary of the following general result.

Theorem 4 (Theorem 2.3.1 of [9]) *The following statements are equivalent:*

- *the discrete Hamiltonian map is of order r, i.e.*

$$\|\boldsymbol{u}_h - \boldsymbol{u}_{h,N}\| + \|\boldsymbol{p}_h - \boldsymbol{p}_{h,N}\| \lesssim h^{1+r};$$

- *the discrete Lagrangian L_d is of order r, i.e.*

$$\left| \int_0^h L(\boldsymbol{u}, \dot{\boldsymbol{u}}, t)\, dt - L_d(\boldsymbol{u}_0, \boldsymbol{u}_h) \right| \lesssim h^{1+r}. \qquad \square$$

Given the boundary values $(\boldsymbol{u}_0, \boldsymbol{u}_h)$ we denote with $\boldsymbol{u} \in X$ and $\boldsymbol{u}_N \in X_N$ the stationary points of $\mathcal{S}$ and $\mathcal{S}_N$ respectively with the constraints:

$$\boldsymbol{u}(0) = \boldsymbol{u}_N(0) = \boldsymbol{u}_0 \quad \text{and} \quad \boldsymbol{u}(h) = \boldsymbol{u}_N(h) = \boldsymbol{u}_h.$$

Clearly such paths are solutions of the principle of least action and represent the path of the mechanical system between the configurations $\boldsymbol{u}_0$ and $\boldsymbol{u}_h$ (in the continuous and discrete settings respectively), their existence and uniqueness can be proved in the same way of Theorem 1 and Theorem 2.

The second statement of Theorem 4 can be recast in the form:

$$|\mathcal{S}(\boldsymbol{u}) - \mathcal{S}_N(\boldsymbol{u}_N)| \lesssim h^{1+r}.$$

Using the triangle inequality the left hand side can be written as:

$$|\mathcal{S}(\boldsymbol{u}) - \mathcal{S}_N(\boldsymbol{u}_N)| \leq |\mathcal{S}(\boldsymbol{u}) - \mathcal{S}(\boldsymbol{u}_N)| + |\mathcal{S}(\boldsymbol{u}_N) - \mathcal{S}_N(\boldsymbol{u}_N)|$$

where the first term depends only on the definition of the space X_N and the second one on the accuracy of the quadrature rule. If we assume that the Lagrangian L is smooth enough, than we can apply the Taylor's theorem, obtaining the identity

$$\mathcal{S}(\boldsymbol{u}_N) - \mathcal{S}(\boldsymbol{u}) = D_{\boldsymbol{u}}\mathcal{S}[\boldsymbol{u}_N - \boldsymbol{u}] + \\ + \int_0^1 (1-s) D^2_{s\boldsymbol{u}_N + (1-s)\boldsymbol{u}} \mathcal{S}[\boldsymbol{u}_N - \boldsymbol{u}, \boldsymbol{u}_N - \boldsymbol{u}]\, ds,$$

where $D_{\boldsymbol{u}}\mathcal{S}$ and $D^2_{\boldsymbol{u}}\mathcal{S}$ denotes respectively the first and second Fréchet derivatives of the functional $\mathcal{S}$. Since $\boldsymbol{u}$ is given by the principle of least action then it is also a solution of Euler–Lagrange equations, then

$$D_{\boldsymbol{u}}\mathcal{S}[\boldsymbol{u}_N - \boldsymbol{u}] = \boldsymbol{p}_h \cdot (\boldsymbol{u}_N - \boldsymbol{u})(h) - \boldsymbol{p}_0 \cdot (\boldsymbol{u}_N - \boldsymbol{u})(0) = 0.$$

Moreover, assuming a Lagrangian of the canonical form with the bilinear form μ bounded and the force field $\boldsymbol{F_u}$ Lipschitz continuous, both uniformly with respect their arguments, then we have

$$D^2_{s\boldsymbol{u}_N+(1-s)\boldsymbol{u}}\mathcal{S}[\boldsymbol{u}_N-\boldsymbol{u},\boldsymbol{u}_N-\boldsymbol{u}] \lesssim \|\boldsymbol{u}_N-\boldsymbol{u}\|^2_X.$$

Therefore, we can conclude with the following theorem.

Theorem 5 *For any boundary conditions $(\boldsymbol{u}_0,\boldsymbol{u}_h)$ and for small enough h, the solutions $\boldsymbol{u}\in X$ and $\boldsymbol{u}_N\in X_N$ satisfy the following estimate:*

$$|\mathcal{S}(\boldsymbol{u})-\mathcal{S}_N(\boldsymbol{u}_N)| \lesssim \|\boldsymbol{u}-\boldsymbol{u}_N\|^2_X + |\mathcal{S}(\boldsymbol{u}_N)-\mathcal{S}_N(\boldsymbol{u}_N)|. \qquad \square$$

5 Discussion of the error estimates

We discuss now the error estimates that can be obtained using the analysis developed in the previous section. We start by noticing that all the results presented in [7, 9, 13, 12] can be recast in the theoretical framework presented in this paper. From now on, the space X_N is the space of polynomials of degree at most N and the quadrature rules are the Gauss or Gauss-Lobatto quadrature with N or $N+1$ nodes. The great advantage of Gauss quadrature is that such rules integrate exactly polynomials of degree $2M-1$ ($2M-3$ for Gauss–Lobatto quadrature) if M nodes are used. Then in the case of Gauss quadrature with $M\geq N$ the norm $\|\cdot\|_X$ is evaluated exactly:

$$\|\boldsymbol{u}_N\|_{X_N} = \|\boldsymbol{u}_N\|_X, \quad \forall \boldsymbol{u}_N\in X_N.$$

The same for Gauss-Lobatto quadrature with $M\geq N+1$ and if $M=N$ the equivalence between the norms $\|\cdot\|_X$ and $\|\cdot\|_{X_N}$ is ensured by [4, Lemma 3.2]:

$$\|\dot{\boldsymbol{u}}_N\|_0 \leq |\dot{\boldsymbol{u}}_N|_{0,N} \leq \sqrt{2+\frac{1}{N}}\|\dot{\boldsymbol{u}}_N\|_0, \quad \forall \boldsymbol{u}_N\in X_N.$$

It is worthwhile noticing that the well-posedness in the last case can not be proved with the theory exposed in [7], as already pointed out in [13]. In fact Lemma 3.1 in [7] states that a quadrature rule with order at least $2N-1$ is only a sufficient condition for the well-posedness. On the other hand Lemma 1 gives also a necessary condition and it can be read as *"the Galerkin variational integrator is well-posed if and only if it is able to solve the free particle equations"*.

The analysis of convergence properties of these methods is more involved. For a while let us assume that all the integral are evaluated exactly then Theorem 3 and Theorem 5 reduce to the inequalities:

$$\|\boldsymbol{u}-\boldsymbol{u}_N\|_X \lesssim \inf_{\boldsymbol{v}_N\in X_N}\|\boldsymbol{u}-\boldsymbol{v}_N\|_X, \quad |\mathcal{S}(\boldsymbol{u})-\mathcal{S}_N(\boldsymbol{u}_N)| \lesssim \|\boldsymbol{u}-\boldsymbol{u}_N\|^2_X,$$

thus the error is bounded by the best approximation error in X. In the case of smooth solutions we obtain [5, Section 5.4]

$$\inf_{\boldsymbol{v}_N\in X_N}\|\boldsymbol{u}-\boldsymbol{v}_N\|_X \lesssim e^{-\gamma N}h^N.$$

Using Theorem 4 the predicted order is $2N-1$. However, as pointed out in [13], at least in the case of a harmonic oscillator with exact quadrature, a higher rate of convergence of order $2N$ is numerically obtained. This suggest that our estimates are not optimal and a deeper analysis is required to better understand the discrepancy between the theoretical estimates and the the numerical results. In the case of less regular solution the best approximation error estimate is given by:

$$\inf_{\boldsymbol{v}_N \in X_N} \|\boldsymbol{u} - \boldsymbol{v}_N\|_X \lesssim N^{-s} h^{\min(s,N+1)-1} |u|_{H^{s;N}(0,h)}, \tag{13}$$

where

$$|u|^2_{H^{s;N}(0,h)} \coloneqq \sum_{k=\min(s,N+1)}^{s} \left\| \frac{d^k u}{dt^k} \right\|_{L^2(0,h)},$$

so that also $|u|_{H^{s;N}(0,h)}$ depends on the value of h and we expect that such dependence is measured by the numerical experiments. In order to provide a more reliable estimate of the error on the interval $(0,h)$ with the proper dependence on h we consider an alternative approach. Instead of considering the mechanical problem defined on the interval $(0,h)$ we consider a fixed interval: without loss of generality we can consider the interval $(0,1)$ divided into K subintervals of measure $h = 1/K$. The idea is to compose the error estimate on each subintervals in order to obtain an estimate for a sub-interval of measure h. Here we analyze two different measures of the error. The first is a rigorous error estimate defined as the maximum on all the subintervals:

$$e_{\max} \coloneqq \max_{i=0,\dots,K-1} \inf_{\boldsymbol{v}_N \in X_{N,i}} \|\boldsymbol{u} - \boldsymbol{v}_N\|_{X_i},$$

where $X_{N,i} = H^1(hi, hi+h)$ and X_N is the space of polynomials of degree at most N on the interval $(hi, hi+h)$. Using the estimate (13) on each subintervals we obtain the estimate

$$e_{\max} \lesssim N^{-s} h^{\min(s,N+1)-1} |u|_{H^{s;N}(0,1)}.$$

This estimate is very conservative, it is valid for all $u \in H^1(0,1)$, in particular it can be considered optimal in the case there exists i such that

$$|u|_{H^{s;N}(0,1)} = |u|_{H^{s;N}(hi,hi+h)}.$$

The second error measure, which is not a real error estimate, but an error *indicator*, is defined as the mean of the errors on all the subintervals:

$$e_{\text{mean}} \coloneqq \frac{1}{K} \sum_{i=0}^{K-1} \inf_{\boldsymbol{v}_N \in X_{N,i}} \|\boldsymbol{u} - \boldsymbol{v}_N\|_{X_i},$$

thus e_{mean} is bounded by

$$e_{\text{mean}} \lesssim N^{-s} h^{\min(s,N+1)-1/2} |u|_{H^{s;N}(0,1)}.$$

The convergence rate for e_{mean} is the same measured in the numerical experiments [13, 12]. Obviously this is not a rigorous bound for the error, but in the particular case in which

$$|u|_{H^{s;N}(hi,hi+h)} = |u|_{H^{s;N}(hj,hj+h)}, \quad \forall i, j \in \{0, \dots, K-1\},$$

the value of e_{mean} is of the same order of $\|\boldsymbol{u} - \boldsymbol{u}_N\|_{X,i}$ for all i.

The estimate $e_{\max}$ gives the lower bound for the order of the Galerkin variational integrators based on polynomials spaces. We expect that the estimate obtained using e_{mean} is better in the practice. Nevertheless it can not be taken to be valid in all cases. Until now we are not able to find an example of mechanical system such that the measured order is equal to the one predicted by $e_{\max}$.

Finally, we want to estimate the error introduced by the quadrature rule. We have to estimate both the consistency error in Theorem 3 and the quadrature order in Theorem 5. In order to estimate the consistency error we use the following estimate of integration error [5, Section 5.4]:

$$\left| \int_0^h f(t)p(t)\,dt - \sum_{k=0}^{M} f(t_k)p(t_k)w_k \right| \lesssim N^{-s} h^{\min(s,M+1)} |f|_{H^{s;M}(0,h)} \|p\|_{L^2(0,h)},$$

which is valid for all polynomial p of degree at most N and for both Gauss–Lobatto quadrature with $M+1$ nodes, where $M+1 \geq N$. Using the Friedrichs' inequality we obtain that the order of the consistency error is smaller than the approximation error. Then we can conclude that the all methods presented in [9, 13, 12] share the same estimate for the error along the path. Moreover, the convergence order predicted by Theorem 3 depends on the regularity of the solution and the polynomial order N, in particular for smooth solutions the order is equal to $N + 1/2$.

Finally we have to estimate the quadrature error in Theorem 5 that determines the order of the method. For both the Gauss and Gauss–Lobatto quadrature the order is determined only by the number of nodes if the integrand function is smooth enough. If we assume a rule with $M+1$ nodes then

$$\left| \int_0^h f(t)\,dt - \sum_{k=0}^{M} f(t_k)w_k \right| \approx \begin{cases} h^{2M+1} & \text{Gauss,} \\ h^{2M-1} & \text{Gauss–Lobatto.} \end{cases}$$

Applying the Theorem 5 to the cases of Gauss quadrature with N nodes and Gauss–Lobatto quadrature with $N+1$ nodes the expected order is $2N-2$ as measured and proved in a different way in [13, 12].

6 Numerical results

In this section, numerical results assessing the convergence properties of Galerkin variational integrators will be presented and discussed. Moreover, in order to show the efficiency of these high-order integrators, the computational cost required by these high order schemes to reach a prescribed error tolerance will be compared with standard low-order schemes.

6.1 Harmonic oscillator

We first consider a simple harmonic oscillator for which the bilinear form and the potential energy in the Lagrangian (2) are given by

$$\mu(\dot{u},\dot{u}) = m\big(\dot{u}(t)\big)^2, \qquad V(t,u) = \frac{1}{2}k\big(u(t)\big)^2,$$

where m is the mass and k is a positive constant defining the restoring force $F = -ku$, while there are no external forces field acting on the system.

The problem is numerically solved in time using the Galerkin variational integrators, considering different polynomial degrees N and Gauss quadrature with $N+1$ nodes. The convergence behavior with respect to the time step h is displayed in Figure 1 (left) for different polynomial degrees. The measured convergence rate is $2N$ confirming the super-convergence discussed in Section 4. The exponential convergence with respect to the polynomial order N has been also assessed, see Figure 1 (right).

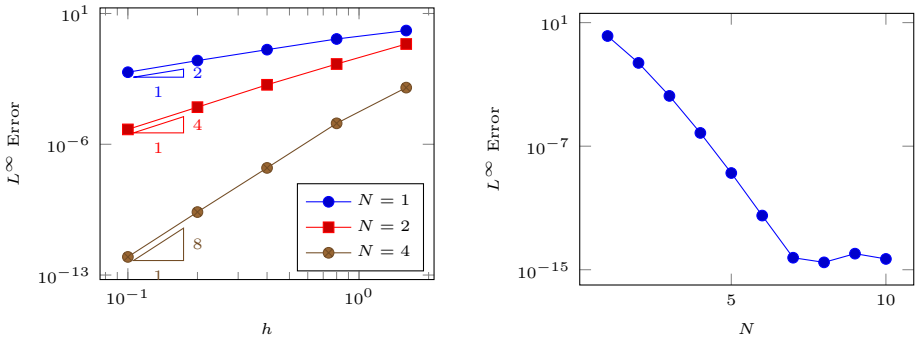

Figure 1: h-convergence (left) and N-convergence (right) for the harmonic oscillator test case.

6.2 Brownout simulations

Brownout is a critical phenomenon experienced by helicopters when landing (or taking off) on sandy soils and consists in a visibility area restriction due to the uplifting of sand particles in the air by vortices of the aerodynamic field. Different models have been proposed in the literature to simulate this phenomenon (see, e.g. [14]). Here we consider a very simple physical model based on non-interacting particles moving in a given aerodynamic velocity field that have been used in [10] to perform brownout simulations (see Figure 2).

The trajectory of a particle with mass m can be computed by the second Newton's law $m\ddot{\boldsymbol{u}} = \boldsymbol{f}$, where $\boldsymbol{u}$ is the position of the particle. The force acting on the particle is given by the drag exerted by the aerodynamic field and by the

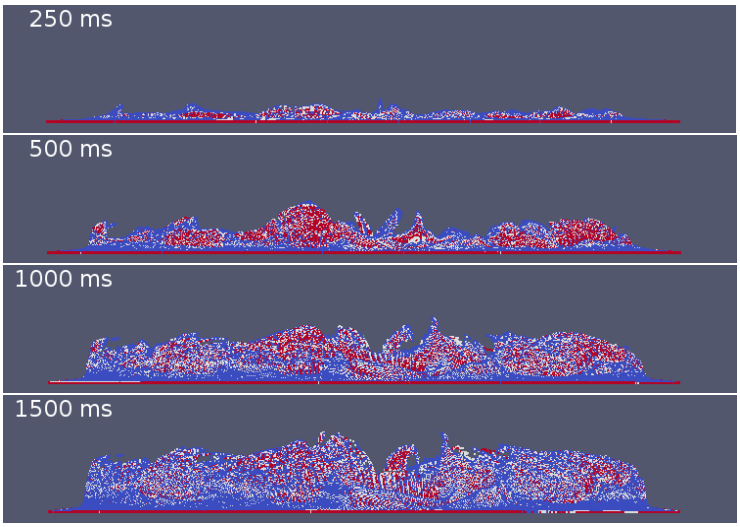

Figure 2: Simulation of the brownout phenomenon: particle distributions at different time instants. Different colors denote different particle sizes.

gravity force, namely:

$$\mathbf{f}(t, \dot{\mathbf{u}}) = -\frac{1}{2}\rho_{air}\|\dot{\mathbf{u}} - \mathbf{v}_{wind}\|(\dot{\mathbf{u}} - \mathbf{v}_{wind})\frac{\pi d^2}{4}C_{\mathrm{d}} - m\mathbf{g}, \tag{14}$$

where $\mathbf{v}_{wind}$ is the wind velocity at the position of the particle, $\mathbf{g}$ is the gravitational acceleration, d is the diameter of the particle, ρ_{air} is the (uniform) air density and C_d is a drag coefficient.

The problem is numerically solved by means of the Galerkin variational integrators with different polynomial degrees. Since the interaction among the particles is not considered in the brownout model, the numerical convergence analysis has been carried out on a single particle dynamics, measuring the L^∞ error on the trajectory with respect to a reference solution obtained with a high polynomial degree ($N = 12$) The convergence behavior with respect to the time step h is displayed in Figure 3 (left), for different polynomial degrees and compared with the solution obtained by a first-order semi-implicit symplectic Euler scheme. The theoretical convergence analysis presented in Section 4 is limited to external forces which are only function of time and position. Nevertheless, the results show that optimal convergence rates can also be obtained when the external force (in this case $\mathbf{F}_p$) depends on the velocity too. Note that the error saturation visible in Figure 3 (left) is due to the tolerance adopted for the convergence of the Newton method used to resolve the nonlinearity in the forcing term.

The same results have been analyzed taking into account the total CPU time required by the different time integrators, in order to investigate the trade-off between the higher rate of convergence of high order schemes and their higher

computational complexity. In Figure 3 (right), the L^∞ error on the trajectory is displayed as a function of the total CPU time required for different integrators. These results clearly show that, when low error level are required, high order variational methods are more efficient than standard low order schemes.

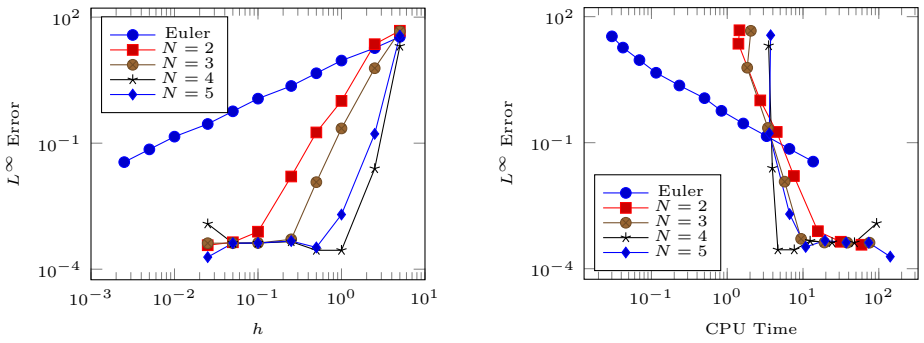

Figure 3: h-convergence for the particle dynamics test case (left) and comparison of CPU times (right).

Conclusions

We have presented a new framework for the definition and analysis of Galerkin variational integrators of arbitrary order. In the presented setting we are able to solve most of the open issues of the Galerkin variational integrator in the case of a Lagrangian of canonical form: we give the necessary and sufficient conditions for the well-posedness and we provide a complete error analysis that includes a justification for the rate of convergence measured in the numerical experiments and not predicted by the standard error analysis. The convergence properties and the computational performance of the proposed time integrators have been assessed through numerical test cases. In particular, particle dynamics simulations for the analysis of brownout phenomena have been carried out proving the effectiveness of the proposed method in reducing the CPU time required to achieve a prescribed level of accuracy in the prediction of particle trajectory.

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