

FRACTIONAL VARIATIONAL INTEGRATORS BASED ON CONVOLUTION QUADRATURE

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ABSTRACT. Fractional dissipation is a powerful tool to study non-local physical phenomena such as damping models. The design of geometric, in particular, variational integrators for the numerical simulation of such systems relies on a variational formulation of the model. In [19], a new approach is proposed to deal with dissipative systems including fractionally damped systems in a variational way for both, the continuous and discrete setting. It is based on the doubling of variables and their fractional derivatives. The aim of this work is to derive higher-order fractional variational integrators by means of convolution quadrature (CQ) based on backward difference formulas. We then provide numerical methods that are of order 2 improving a previous result in [19]. The convergence properties of the fractional variational integrators and saturation effects due to the approximation of the fractional derivatives by CQ are studied numerically.

1. INTRODUCTION

Fractional calculus is an extension of classical integration and differentiation theory to any real or complex order [3], [33], [34], [36]. A major feature enjoyed by fractional calculus is non-locality which is used widely to model numerous phenomena in mechanics and physics. Fractional damping systems including dissipation can be considered as a variational problem with a Lagrangian which depends on fractional derivatives, so that the corresponding equations of motion arise from Hamilton's principle. In this context, a new variational approach, the so-called *restricted Hamilton's principle* was developed by Jiménez and Ober-Blöbaum [19]. Contrary to the classical Hamilton's principle, the restricted one gives only *sufficient* conditions for the extremals of the fractional variational problem leading to *restricted fractional Euler-Lagrange equation*:

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = -\mu D_-^\alpha x, \quad \mu > 0, \quad \alpha \geq 0 \quad (1)$$

where $L(t, x, \dot{x})$ is a Lagrangian and D_-^α is the fractional derivative operator.

There are several interesting applications of the fractional dynamical equation (1). For example, it can be used to describe the dynamics of damped linear system when $\alpha = 1$, i.e. the fractional derivative becomes the full derivative or the motion of rigid plate immersed in a Newtonian fluid for fractional derivatives of order $3/2$ [37].

Dealing with variational problems permit us to construct variational integrators [15], [28] via a discrete calculus of variations which are numerical schemes for Lagrangian systems preserving their variational structures. For this purpose, it is important to derive of the equations of motion for forced systems (equation (1) with $\alpha = 1$) in a purely variational way. There exist several attempts in this direction, some of those based on duplicating the variables of the system [10], [14]. The construction of the desired forced variational integrators was motivated by [10].

The notion of variational integrators to the fractional case has been discussed [18] using a discrete restricted Hamilton's principle. This approach based on the Grünwald-Letnikov approximation of the fractional derivatives, is also developed in [19]. Such approximation has been proved

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to be of order one consistency, so that the convergence order the resulting scheme, called *Fractional Variational Integrator* (FVI) is then limited by 1. Following the previous work [19], our purpose is to derive high-order variational integrators for (1) by combining high-order variational techniques [30], [31] with *convolution quadrature* (CQ) [24], [26].

Among several numerical methods used in the fractional framework, convolution quadrature preserves structure. More concretely, there are two important properties of fractional operators used in the restricted Hamilton's principle: integration by parts and semigroup properties. For the construction of FVI, preserving such properties at the discrete setting is then essential which can be done by CQ.

Convolution quadrature was introduced by Lubich [24], [26]. This method is a numerical tool for approximating convolution integral by a specific quadrature rule. The main difference between this method and other numerical methods is that the weights of CQ are computed by Laplace transform of the convolution kernel and multistep methods. For the *left* fractional integral, which is a particular convolution integral, the quadrature weights are obtained from the fractional order power of the rational polynomial of the generating functions of LMMs. In particular, the use of backward difference formulas (BDFs) is a subclass of LMMs which is widely adopted for high accuracy [22], [23].

The FVIs is mainly a combination of two different algorithms: one for fractional part and the other for conservative part. As we deal with higher order approximation, the above listed strategy is appropriate for the fractional derivative involved in (1). Besides that, it is also natural to apply higher order approximation for the conservative part and this motivates us to use high-order variational techniques.

High-order variational techniques, also known as high-order variational integrators or Galerkin variational methods are numerical approaches applied to the action integral associated to a Lagrangian L in order to construct numerical schemes of arbitrarily high order. It is based on interpolating the trajectories and choosing a high-order quadrature for the approximation of the integral, see [20], [28], [31] and references therein.

The work is organized as follows. In Section 2 we give a brief exposition of Lagrangian variational integrators that will be used throughout the work. Section 3 contains some necessary preliminaries of fractional calculus, and we present the notion of convolution quadrature, in particular, Lubich's fractional linear multi-step methods. We also discuss the main issue of using convolution quadrature together based on BDFs with numerical experiments as illustration. After recalling a continuous restricted Hamilton's principle in Section 4, we present our new contribution as a generalisation of the one obtained by [19] for deriving FVIs associated to (1) by means of the convolution quadrature in the framework of the discrete restricted Hamilton's principle. We examine the accuracy of such integrators using the damped oscillator and the Bagley-Torvik problems. The final Section we treat the case higher order FVIs by applying high-order techniques as presented in [30], [31] mixed with convolution quadrature to obtain higher order fractional variational integrators.

2. HIGHER ORDER DISCRETE VARIATIONAL MECHANICS

In this section, we remind the construction of variational integrators which will be used in this work. We refer to [20], [28], [31] and references therein for more details.

2.1. Hamilton's principle and Euler-Lagrange equations. Consider a mechanical system defined on the d -dimensional configuration manifold Q (later on we will particularize on \mathbb{R}^d , but in this section it can be considered as a general smooth manifold) with corresponding tangent bundle TQ . Let $q(t) \in Q$ and $\dot{q}(t) \in T_{q(t)}Q$, $t \in [0, T] \subset \mathbb{R}$, $0 < T$, be the time-dependent

configuration and velocity of the system. The action $S : C^2([0, T], Q) \rightarrow \mathbb{R}$ of a mechanical system is defined as the time integral of the Lagrangian, i.e.

$$\mathcal{L}(q) = \int_0^T L(q(t), \dot{q}(t)) dt, \quad (2)$$

where the C^2 Lagrangian function $L : TQ \rightarrow \mathbb{R}$ consists of kinetic minus potential energy. Hamilton's principle seeks curves q , with fixed initial and final values $q(0)$ and $q(T)$, which are *extremals* of the action, i.e. satisfying

$$\delta \mathcal{L}(q) = 0,$$

for arbitrary variations $\delta q \in T_q C^2([0, T], Q)$. A necessary and sufficient condition for the extremals is the so-called Euler-Lagrange equation

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0, \quad (3)$$

which are a second-order differential equation and describes the dynamics of conservative systems. See [1] for more details.

2.2. Discrete Hamilton's principle and discrete Euler-Lagrange equations. The discretization of the objects described in the previous subsection is based on [28], [29]. Let us consider a time grid $t_k = \{k h \mid k = 0, \dots, N\}$, where $h \in \mathbb{R}_+$ is the time step and $hN = T$. We replace the configuration $q(t)$ by a discrete sequence $q_d \equiv \{q_k\}_{0:N} \in Q^{N+1}$ where q_k will be an approximation of $q(t_k)$. The discrete Lagrangian $L_d : Q \times Q \rightarrow \mathbb{R}$ will be an approximation of the action (2) in one time step $[t_k, t_{k+1}]$ based on two neighboring configurations q_k and q_{k+1} , i.e.

$$L_d(q_k, q_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(q(t), \dot{q}(t)) dt. \quad (4)$$

Furthermore, the discrete action sum $\mathcal{L}_d : Q^{N+1} \rightarrow \mathbb{R}$ is defined by

$$\mathcal{S}_d(q_d) = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}).$$

The discrete Hamilton's principle seeks extremals of the action \mathcal{L}_d with fixed endpoints q_0, q_N , i.e.

$$\delta \mathcal{S}_d(q_d) = 0,$$

for arbitrary $\delta q_k \in T_{q_k} Q$. A necessary and sufficient condition for the extremals are the discrete Euler-Lagrange equations

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0, \quad k = 1, \dots, N-1, \quad (5)$$

where D_i is the derivative with respect to the i -th argument. Given that the matrix $D_{12} L_d(q_k, q_{k+1})$ is regular, equation (5) provides a discrete iteration scheme for (3) that determines q_{k+1} for given q_k and q_{k-1} . This iteration scheme, that can be represented by the map $F_{L_d} : Q \times Q \rightarrow Q \times Q$, $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$, is called *variational integrator*, and has interesting preservation properties, such as symplecticity and momentum preservation under the action of a symmetry [28], [29].

2.3. Higher order approximations of the action. Considering only two neighboring configurations q_k and q_{k+1} in (4) limits the approximation order to $O(h^2)$. With the aim of increasing this order, a well-known approach is to take into account inner nodes in between $[t_k, t_{k+1}]$ [16], [28], [31]. This higher order approximation procedure consists of two steps: (1) the approximation of the space of trajectories and (2) the approximation of the integral of the Lagrangian by appropriate quadrature rules.

(1) *Trajectories space.* The space $\mathcal{C}([t_k, t_{k+1}], Q) = \{q : [t_k, t_{k+1}] \rightarrow Q \mid q(t_k) = q_k, q(t_{k+1}) = q_{k+1}\}$, will be approximated by $\mathcal{C}^s([t_k, t_{k+1}], Q) \subset \mathcal{C}([t_k, t_{k+1}], Q)$, where $\mathcal{C}^s([t_k, t_{k+1}], Q)$ denotes the space of polynomials of degree s . Given $s+1$ control points $0 = d_0 < d_1 < \dots < d_{s-1} < d_s = 1$ and $s+1$ configurations $q_k = (q_k^0, q_k^1, \dots, q_k^{s-1}, q_k^s)$, with $q_k^0 = q_k$ and $q_k^s = q_{k+1}$, then $q_d(t; k) \in \mathcal{C}^s([t_k, t_{k+1}], Q)$ can be defined by

$$q_d(t; k) = \sum_{\nu=0}^s q_k^\nu \ell_\nu \left(\frac{t}{h} \right), \quad (6)$$

where $\ell_\nu(\tau)$ are Lagrange polynomials of degree s such that $\ell_\nu(d_i) = \delta_{\nu i}$ (here δ is the Kronecker symbol), and therefore $q_d(h d_i; k) = q_k^i$ according to (6). Moreover, the time derivative of (6) is

$$\dot{q}_d(t; k) = \frac{1}{h} \sum_{\nu=0}^s q_k^\nu \dot{\ell}_\nu \left(\frac{t}{h} \right).$$

(2) *Quadrature for the action integral.* For the approximation of the action integral (2), first we replace the curves $q(t)$ and $\dot{q}(t)$ by their polynomial counterparts $q_d(t; k)$, $\dot{q}_d(t; k)$ in the interval $[kh, (k+1)h]$, i.e.

$$\int_{kh}^{(k+1)h} L(q_d(t; k), \dot{q}_d(t; k)) dt, \quad k = 0, \dots, N-1.$$

Next, in the same time interval, a quadrature rule $(b_i, c_i)_{i=1}^r$ is applied, with $c_i \in [0, 1]$. This defines the discrete Lagrangian:

$$L_d(q_k) \equiv L_d(q_k^0, \dots, q_k^s) := h \sum_{i=1}^r b_i L(q_d(c_i h; k), \dot{q}_d(c_i h; k)); \quad (7)$$

it is important to remark that L_d depends on $s+1$ variables. Naturally, the choice of quadrature should be adapted to the desired order of approximation with respect to the continuous action in order that now can be arbitrarily high.

The construction of higher order variational integrators can be summarized in Figure 1.

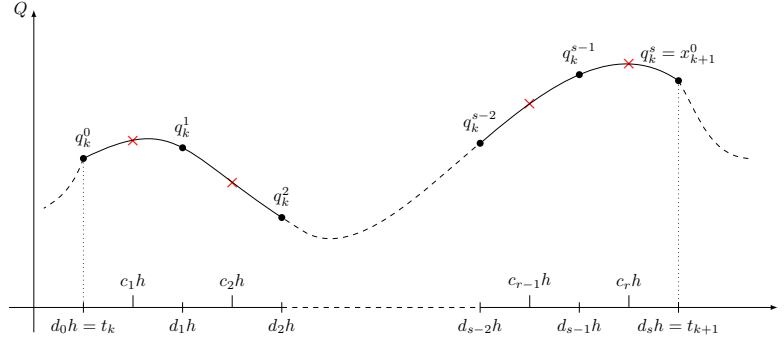


Figure 1. Polynomial interpolation principles. On each subinterval $[t_k, t_{k+1}]$, the trajectory interpolated by a polynomial passing through the points $\{q_k^i\}_{i=0}^s$ associated with the control points $\{d_\nu h\}$. The evaluations are made by the quadrature points for the $\{c_i h\}$, indicated by cross points.

Now, following §2.2, the action sum can be defined from (7) by

$$\mathcal{S}_d(q_d) = \sum_{k=0}^{N-1} L_d(q_k),$$

and the discrete Hamilton's principle can be applied in order to obtain a necessary and sufficient condition for its extremals, i.e. the discrete Euler-Lagrange equations. These are:

$$\begin{aligned} D_{s+1}L_d(q_{k-1}^0, \dots, q_{k-1}^s) + D_1L_d(q_k^0, \dots, q_k^s) &= 0, \\ D_iL_d(q_k^0, \dots, q_k^s) &= 0, \quad \forall i = 2, \dots, s; \end{aligned}$$

for $k = 1, \dots, N-1$, where the transition condition, namely $q_{k-1}^s = q_k^0$ has to be taken into account. See [28], [31] for further details.

Higher order variational integrators (also denoted as Galerkin variational integrators) have been extensively studied in [7], [16], [20], [31] for conservative systems and in [8] for optimal control problems. Obviously, the convergence order of higher order variational integrators is limited by the order of the function space approximation and the order of the quadrature rule. In [16] a lower error bound is provided by the approximation order of the finite-dimensional function space (e.g. convergence order s is reached by using the space of polynomials of degree s). Numerical convergence studies in [31] indicate that Galerkin variational integrators based on the Lobatto and Gauss quadrature rules are of order $\min(2s, u)$, where s is the degree of the polynomial and u the order of the quadrature rule. A general proof of this superconvergence result is provided in [32] using backward error analysis in the context of the calculus of variations. For particular classes that are equivalent to so-called (modified) symplectic Runge-Kutta methods, a proof of a superconvergence has been made in [30].

3. FRACTIONAL INTEGRALS, FRACTIONAL DERIVATIVES AND THEIR APPROXIMATIONS BY DISCRETE CONVOLUTIONS

3.1. Fractional integrals and fractional derivatives. Let us start by giving a brief overview concerning the fractional operators. We refer to [3], [33], [36] for more details.

3.1.1. Fractional integrals. The Riemann-Liouville α -fractional integrals, $\operatorname{Re} \alpha > 0$, for $f : [0, T] \rightarrow \mathbb{R}^1$ are defined by

$$J_-^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} f(\tau) d\tau, \quad t \in (0, T], \quad (8a)$$

$$J_+^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_t^T (\tau - t)^{\alpha-1} f(\tau) d\tau, \quad t \in [0, T], \quad (8b)$$

where Γ is the Euler Gamma function and we set $J_-^0 f = J_+^0 f = f$. The fractional integrals satisfy the so-called *semigroup property* [36, Theorem 2.5, p.46], i.e.

$$J_\sigma^\alpha J_\sigma^\beta f(t) = J_\sigma^{\alpha+\beta} f(t), \quad \sigma \in \{-, +\}. \quad (9)$$

Let $m \in \mathbb{N}$. If the function f is continuously differentiable in $[0, T]$, then it can be continued analytically to $\operatorname{Re} \alpha < 0$ via

$$J_-^\alpha f(t) = \frac{d^m}{dt^m} J_-^{m+\alpha} f(t), \quad J_+^\alpha f(t) = \frac{d^m}{dt^m} J_+^{m+\alpha} f(t) \quad \text{for } \operatorname{Re} \alpha > -m. \quad (10)$$

In this case, the fractional integral is called *fractional derivative*, and can be denoted by $D^{-\alpha}$ (note that the real part of α is now negative).

In particular, from (10), and restricting ourselves to $\operatorname{Re} \alpha \in [0, 1]$ (which will be the range of interest in this work), we can establish the following definition of Riemann-Liouville fractional derivatives, which is usually found in the literature:

¹For $f \in L^1([0, T]; \mathbb{R})$, $J_-^\alpha f$ and $J_+^\alpha f$ are defined almost everywhere on $[0, T]$. Moreover, they are defined everywhere on $[0, T]$, if $f \in C([0, T]; \mathbb{R})$. (see [11], [21], [33] for more details).

3.1.2. *Fractional derivatives.* Let $\operatorname{Re} \alpha \in [0, 1]$. The left and right Riemann–Liouville fractional derivatives are respectively defined by

$$\begin{aligned} D_-^\alpha f(t) &= \frac{d}{dt} J_-^{1-\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-\tau)^{-\alpha} f(\tau) d\tau, \quad t \in (0, T], \\ D_+^\alpha f(t) &= -\frac{d}{dt} J_+^{1-\alpha} f(t) = -\frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_t^T (\tau-t)^{-\alpha} f(\tau) d\tau, \quad t \in [0, T), \end{aligned} \quad (11)$$

provided that $f \in AC([0, T], \mathbb{R})$ which is a very simple sufficient condition for the existence. It is easy to see that $D_-^0 f = D_+^0 f = f$, whereas it can be proven that

$$D_-^1 f = -D_+^1 f = df/dt. \quad (12)$$

The last relationships follow easily from the definitions (11) (first equality) and $J_-^0 f = J_+^0 f = f$, but the latter are not trivial from the definitions (8)².

Other relevant properties of fractional derivatives are

$$\int_0^T f(t) D_\lambda^\alpha g(t) dt = \int_0^T g(t) [D_{-\lambda}^\alpha f(t)] dt, \quad \sigma \in \{-, +\}, \quad (13a)$$

$$D_\lambda^\alpha D_\lambda^\beta = D_\lambda^{\alpha+\beta}, \quad 0 \leq \alpha, \beta \leq 1/2. \quad (13b)$$

Property (13a) is called “asymmetric integration by parts” of the fractional derivatives, whereas (13b) is called again the “semigroup property”.

Remark 3.1. It is important to note that, contrary to the Caputo derivatives, the Riemann–Liouville derivatives of a function f , in particular $D_-^\alpha f(t)$, could lead to singularity at $t = 0$. That is why the Caputo derivatives are more useful in applications, otherwise we should impose $f(0) = 0$, which will be the case in our discussion in Section 4.

3.2. **Fractional integrals as convolutions.** For the time being, let us focus on the *retarded* fractional integral in (8), i.e. $J_-^\alpha f(t)$. It is easy to see that it is a particular convolution integral

$$J_-^\alpha f(t) = (\kappa^{(\alpha)} * f)(t) := \int_0^t \kappa^{(\alpha)}(t-\tau) f(\tau) d\tau \quad (14)$$

where the convolution kernel is given by

$$\kappa^{(\alpha)}(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}. \quad (15)$$

Here, (α) must not be understood as a power in the left hand side, it is just a superscript denoting the dependence of the kernel on the parameter α .³ The Laplace transform of this convolution kernel is given by

$$K^{(\alpha)}(s) := \mathcal{L}(\kappa^{(\alpha)})(s) = \int_0^\infty \frac{t^{\alpha-1}}{\Gamma(\alpha)} e^{-st} dt = s^{-\alpha}. \quad (17)$$

²The expression of the fractional derivative as a fractional integral of negative α -index (and therefore its inverse operator) can be made explicit. Namely, from (9), (11) and (12), plus considering that J_-^1 is the usual integral operator (inverse of the derivative), we have

$$D_-^\alpha f = D_-^1 J_-^{1-\alpha} f = D_-^1 J_-^1 J_-^{-\alpha} f = J_-^{-\alpha} f,$$

where, recall, $\alpha \in [0, 1]$. A similar computation can be done for the Caputo definition of the fractional derivative [36], i.e. ${}_c D_-^\alpha f := J_-^{1-\alpha} D_-^1 f = D_-^\alpha f$ by imposing that $f(0) = 0$.

³In complete generality, a convolution integral can be defined for any kernel as

$$(\kappa * f)(t) := \int_0^t \kappa(t-\tau) f(\tau) d\tau. \quad (16)$$

3.3. Discrete convolution. The theory of discrete convolutions is developed in [24]–[26] by Ch. Lubich (indeed, the topic of [26] is the discretization of fractional integrals).

As in §2.2, let us consider a time grid $t_k = \{kh \mid k = 0, \dots, N\}$, where $h \in \mathbb{R}_+$ is the time step and $hN = T$. Moreover, consider a discrete series $\{f_k\}_{0:N} \in (\mathbb{R}^d)^{N+1}$, where f_k shall be an approximation of $f(t_k)$.

Now, define the discrete convolution in the following as an approximation of the continuous convolution $(\kappa * f)(t_k)$ in (16), namely

$$(\kappa * f)(t_k) \approx (\omega * f)(t_k) := \sum_{n=0}^{\infty} \omega_n f_{k-n} \stackrel{!}{=} \sum_{n=0}^k \omega_n f_{k-n}, \quad (18)$$

observe that the series is truncated after $\stackrel{!}{=}$ since f_k is not defined for $k < 0$ ⁴, with a general convolution kernel κ . The convolution quadrature weights ω_n are defined as the coefficients of the generating power series

$$K\left(\frac{\gamma(z)}{h}\right) := \sum_{n=0}^{\infty} \omega_n z^n, \quad |z| \text{ small}. \quad (19)$$

Here, $K(s)$ is the Laplace transform of the kernel κ and the so-called characteristic function $\gamma(z) = \sum_{n=0}^{\infty} \gamma_n z^n$ is the quotient of the generating polynomials (ρ, σ) of a linear multistep method (LMM)

$$\rho_0 y_k + \rho_1 y_{k-1} + \dots + \rho_n y_{k-n} = h(\sigma_0 f_k + \sigma_1 f_{k-1} + \dots + \sigma_n f_{k-n})$$

for the differential equation $y' = f(y)$, i.e.

$$\gamma(z) = \frac{\rho(z)}{\sigma(z)} = \frac{\rho_0 + \rho_1 z + \dots + \rho_n z^n}{\sigma_0 + \sigma_1 z + \dots + \sigma_n z^n}, \quad (20)$$

where we assume that $\rho_0/\sigma_0 > 0$, so that (19) is well-defined at least for sufficiently small h . Note that if we define z_- to be the discrete backward operator, i.e.

$$z_- f_k = f_{k-1},$$

then the LMM can be defined as $\rho(z_-) y_k = h \sigma(z_-) f_k$, where $\{y_k\}_{0:N} \in (\mathbb{R}^d)^{N+1}$ is also a discrete series.

More importantly for the purposes of this article, the discrete convolution approximating the fractional integral (8a),(14) can be redefined, according to (19), by

$$\mathcal{J}_-^\alpha f_k := K^{(\alpha)}\left(\frac{\gamma(z_-)}{h}\right) f_k = \sum_{n=0}^k \omega_n^{(\alpha)} f_{k-n}, \quad (21)$$

where $K^{(\alpha)}(\gamma(z)/h)$, with $K^{(\alpha)}$ given in (17), has to be understood as an operator acting on $\{f_k\}_{0:N}$. On the other hand, considering the discrete forward operator

$$z_+ f_k = f_{k+1},$$

the discrete convolution approximating the fractional integral (8b) will be

$$\mathcal{J}_+^\alpha f_k := K^{(\alpha)}\left(\frac{\gamma(z_+)}{h}\right) f_k = \sum_{n=0}^{N-k} \omega_n^{(\alpha)} f_{k+n}, \quad (22)$$

⁴It could be argued that a more natural expression for the discrete convolution would be

$$(\omega * f)(t_k) := \sum_{n=0}^k \omega_{k-n} f_n,$$

according to (14) and the relationship between the continuous and discrete times. It can be shown easily that both expressions are equivalent after rearranging the discrete time index and reordering the coefficients. Moreover, (18) will make more sense when the discrete convolution is understood as the application of a certain operator over the discrete series $\{f_k\}_{0:N}$

where again the series (19) gets truncated because $\{f_k\}_{0:N}$ is undefined for $k > N^5$. It is interesting to note that, following these definitions, the convolution weights $\omega_n^{(\alpha)}$ are the same for \mathcal{J}_-^α and \mathcal{J}_+^α .

Now we are in situation to show the proof of some properties relevant for future results.

Lemma 3.1. *Consider two discrete series $\{f_k\}_{0:N}, \{g_k\}_{0:N}$. Then the following properties hold true:*

- (1) *The semigroup property of the discrete convolution: $\mathcal{J}_\lambda^\alpha \mathcal{J}_\lambda^\beta f_k = \mathcal{J}_\lambda^{\alpha+\beta} f_k$.*
- (2) *The asymmetric integration by parts:*

$$\sum_{k=0}^N g_k (\mathcal{J}_-^\alpha f_k) = \sum_{k=0}^N (\mathcal{J}_+^\alpha g_k) f_k. \quad (23)$$

Proof. (1) From the definitions (21) and (22) (first equalities) with $K^{(\alpha)}(s) = s^{-\alpha}$ (17), it follows:

$$\begin{aligned} \mathcal{J}_\lambda^\alpha \mathcal{J}_\lambda^\beta f_k &= K^{(\alpha)} \left(\frac{\gamma(z_\lambda)}{h} \right) K^{(\beta)} \left(\frac{\gamma(z_\lambda)}{h} \right) f_k \\ &= \left(\frac{\gamma(z_\lambda)}{h} \right)^{-\alpha} \left(\frac{\gamma(z_\lambda)}{h} \right)^{-\beta} f_k \\ &= \left(\frac{\gamma(z_\lambda)}{h} \right)^{-\alpha-\beta} = K^{\alpha+\beta} \left(\frac{\gamma(z_\lambda)}{h} \right) = \mathcal{J}_\lambda^{\alpha+\beta} f_k, \end{aligned}$$

(2) See [6] for more details:

$$\begin{aligned} \sum_{k=0}^N g_k (\mathcal{J}_-^\alpha f_k) &\stackrel{=1}{=} \sum_{k=0}^N \sum_{n=0}^k \omega_n^{(\alpha)} g_k f_{k-n} \stackrel{=2}{=} \sum_{n=0}^N \sum_{k=n}^N \omega_n^{(\alpha)} g_k f_{k-n} \\ &\stackrel{=3}{=} \sum_{n=0}^N \sum_{k=0}^{N-n} \omega_n^{(\alpha)} g_{k+n} f_k \stackrel{=4}{=} \sum_{k=0}^N \sum_{n=0}^{N-k} \omega_n^{(\alpha)} g_{k+n} f_k \stackrel{=6}{=} \sum_{k=0}^N (\mathcal{J}_+^\alpha g_k) f_k. \end{aligned}$$

In $=^1$ the definition (21) (second equality) is used. To prove $=^2$ is enough to notice that, for fixed $j = 0, \dots, N$, the elements $a_i := \omega_i^{(\alpha)} g_j f_{j-i}$, $i = 0, \dots, j$, on the left hand side, disposed in columns, form an upper diagonal $(N+1) \times (N+1)$, whereas the same elements on the right hand side, for $j = 0, \dots, N$ and $i = j, \dots, N$, account for the transposed matrix; therefore their total sums are equal. In $=^3$ the sum index is rearranged. In $=^4$ equivalent arguments to $=^2$ can be used. Finally, in $=^6$ the definition (22) (second equality) is used; this concludes the proof. \square

Now, we take into consideration the convergence order of $\mathcal{J}_\lambda^\alpha$ with respect to J_λ^α following [26]; as we will see, this order is sensitive to the convergence order of the multistep method (ρ, σ) . In particular, for the generating function $\gamma = \rho/\sigma$, which gives rise to $\omega_n^{(\alpha)}$ according to (21), we say that the corresponding multistep method is convergent of order p if and only if

$$\tilde{\gamma}_n \text{ are bounded, (stability)} \quad (24a)$$

$$h \tilde{\gamma}(e^{-h}) = 1 + O(h^p), \text{ as } h \rightarrow 0, \text{ (order } p \text{ consistency)}, \quad (24b)$$

where $\tilde{\gamma}_n$ are coefficients of the power series $\gamma^{-1}(z) := 1/\gamma(z)$. Now, we introduce the notion of convergence of the quadrature $\omega_n^{(\alpha)}$.

Definition 3.1. A convolution quadrature determined by the coefficients $\omega_n^{(\alpha)}$ is convergent of order p (to J_λ^α) if

$$J_\lambda^\alpha t^{\beta-1} - \mathcal{J}_\lambda^\alpha t^{\beta-1} = O(h^\beta) + O(h^p), \quad (25)$$

for all $\beta \in \mathbb{C}$, $\beta \neq 0, -1, -2, \dots$.

⁵For a given function, the discrete convolution can be also defined in continuous time, namely

$$\mathcal{J}_\lambda^\alpha f(t) := K^{(\alpha)}(\gamma(z_\lambda)/h) f(t) = \sum_{n \geq 0} \omega_n^{(\alpha)} f(t \pm nh).$$

Theorem 3.1 (Theorem 2.6 in [26]). *Let (ρ, σ) denote an implicit linear multistep method which is convergent of order p (24) and assume that the zeros of σ have absolute value less than 1. Then, $\mathcal{J}_\lambda^\alpha$ (21), (22) are convergent of order p (Definition 3.1) to J_λ^α (8).*

In [26] is also established, under the condition of p -convergence in Definition 3.1, that for functions $f(t) = t^{\beta-1}g(t)$, $g(t)$ smooth, there always exists a starting quadrature $\varpi_{k,n}$ ⁶ which is defined by

$$\tilde{\mathcal{J}}_-^\alpha f_k := \sum_{n=0}^k \omega_n^{(\alpha)} f_{k-n} + h^\alpha \sum_{n=0}^s \varpi_{k,n} f_n, \quad (26)$$

with s fixed, such that

$$J_\lambda^\alpha f - \tilde{\mathcal{J}}_-^\alpha f = O(h^p), \quad (27)$$

uniformly for $t \in [0, T]$. In other words, to achieve the order p convergence of the underlying LMM, the extra term in (27) should be introduced in order to eliminate low order terms in the error bound in (25).

It is important to remark that due to the presence of the extra ϖ -initial terms in (26) the *convolution structure* is violated, and therefore the properties proved in Lemma 3.1 are no longer true for $\tilde{\mathcal{J}}_-^\alpha f$. In Lubich's own words: “*The convolution structure is only violated by the few correction terms of the starting quadrature which will be necessary for high order schemes*”. Indeed, this is also relevant in terms of the convergence order, since from Definition 3.1, Theorem 3.1 and (27) we conclude that for a function $f(t) = t^{\beta-1}g(t)$, with $g(t)$ smooth, a multistep method (ρ, σ) is p -convergent would generate the following convergence bound:

$$J_\lambda^\alpha f - \mathcal{J}_\lambda^\alpha f = O(h^\beta) + O(h^p). \quad (28)$$

Thus, we expect the saturation of the convergence order at $\min(\beta, p)$. We illustrate the saturation (28) for the functions $t \mapsto t^{\beta-1} \sin(t)$, $\beta = 1, 3, 4, 5$ in Figure 2, which is a log-plot of h versus the error e_h , defined as usual in the literature by means of the maximum norm, i.e.

$$e_h = \max_{0 \leq k \leq N} |J_-^\alpha f(t_k) - \mathcal{J}_-^\alpha f_k|, \quad (29)$$

where the h -dependence of e_h is implicit in the time grid t_k . Of our interested, the characteristic function $\gamma(z_-)$ of the classical backward differentiation formula (BDF) up to order 6, that is,

$$\gamma(z) = \sum_{k=1}^p \frac{1}{k} (1-z)^k := \gamma_p(z). \quad (30)$$

⁶In practice, computing $\varpi_{k,n}$ becomes more complicated for some values of α where a linear system should be solved at each step.

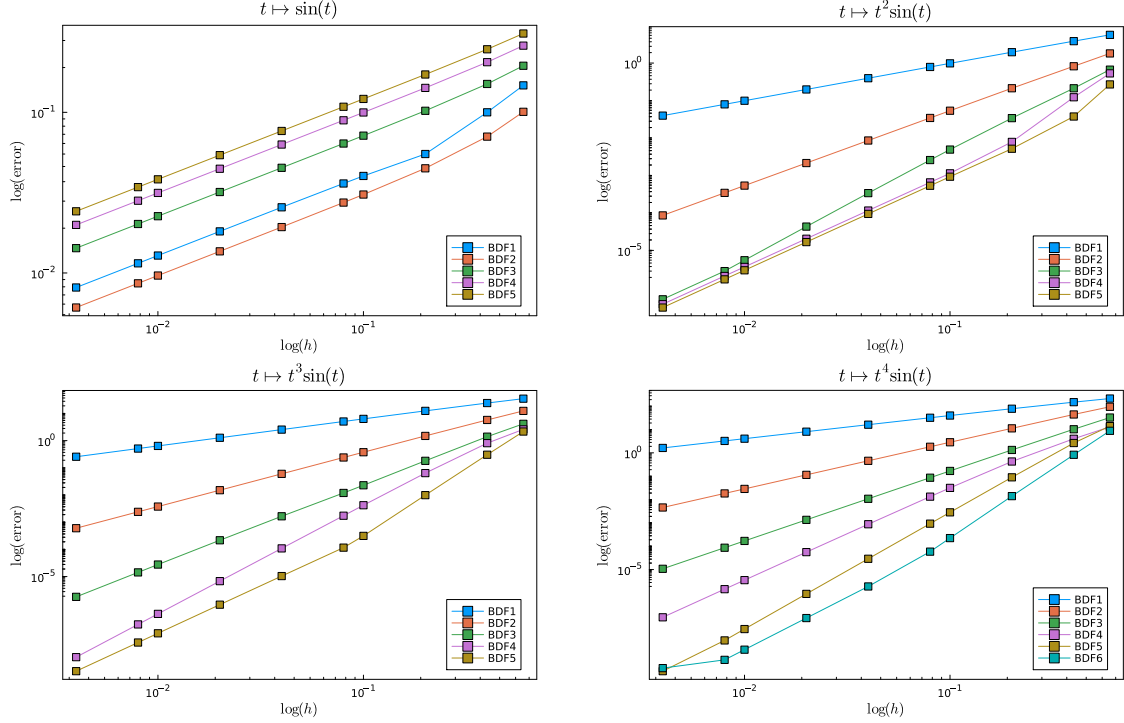


Figure 2. Log-Log plot the error $e(h)$ versus h corresponds to the Caputo fractional derivative of order $1/2$ ($\alpha = -1/2$ in (29)). As expected, the convergence starts to saturate at $p = 1$ (upper-left), $p = 3$ (upper-right), $p = 4$ (lower-left) and $p = 5$ (lower-right).

4. RESTRICTED VARIATIONAL PRINCIPLE FOR THE DYNAMICS OF LAGRANGIAN SYSTEMS SUBJECT TO FRACTIONAL DAMPING

In [18], [19] a restricted variational principle (both continuous and discrete) in order to obtain the dynamics of a Lagrangian system subject to fractional damping is delivered. As in other previous approaches treating dissipative systems in a variational fashion [2], [5], [9], [14], [35], it is based on the doubling of variables and the introduction of their fractional derivatives (which in this work will be considered as fractional integrals with negative α index, as explained in §3) in the state space of the relevant Lagrangians.

4.1. Continuous setting. Let us consider the AC^2 curves $x, y : [0, T] \rightarrow \mathbb{R}^d$ and a C^2 Lagrangian function $L : T\mathbb{R}^d \rightarrow \mathbb{R}$ (also $L : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$). Define a C^2 Lagrangian function⁷

$$\begin{aligned} \mathcal{L} : \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d &\rightarrow \mathbb{R} \\ (x, y, \dot{x}, \dot{y}, J_-^{-\alpha} x, J_+^{-\beta} y) &\mapsto \mathcal{L}(x, y, \dot{x}, \dot{y}, J_-^{-\alpha} x, J_+^{-\beta} y) \end{aligned} \quad (31)$$

$$\mathcal{L}(x, y, \dot{x}, \dot{y}, J_-^{-\alpha} x, J_+^{-\beta} y) = L(x, \dot{x}) + L(y, \dot{y}) - \mu J_-^{-\alpha} x J_+^{-\beta} y,$$

⁷In [18], [19] the state space of \mathcal{L} is defined as a particular vector bundle with base point (x, y) and fiber $(\dot{x}, \dot{y}, J_-^{-\alpha} x, J_+^{-\beta} y)$. However, this space is totally isomorphic to the Cartesian product of six copies of \mathbb{R}^d and we will stick to this for simplicity, preserving the notation of the base point (x, y) as argument of the forthcoming actions also for simplicity.

where $\alpha, \beta \in [0, 1/2]$ and $\mu \in \mathbb{R}_+$. Given this particular Lagrangian, we define the relevant action:

$$\begin{aligned} \mathcal{S}(x, y) &= \mathcal{S}^{\text{cons}}(x, y) + \mathcal{S}^{\text{frac}}(x, y), \\ \mathcal{S}^{\text{cons}}(x, y) &= \int_0^T (L(x(t), \dot{x}(t)) + L(y(t), \dot{y}(t))) dt, \quad \mathcal{S}^{\text{frac}}(x, y) = -\mu \int_0^T J_-^{-\alpha} x(t) J_+^{-\beta} y(t) dt, \end{aligned} \quad (32)$$

where *cons* goes after “conservative” and *frac* after “fractional”. Moreover, let us define restricted varied curves by means of

$$x_\epsilon(t) = x(t) + \epsilon \delta x(t), \quad y_\epsilon(t) = y(t) + \epsilon \delta x(t), \quad (33)$$

with $\epsilon \in \mathbb{R}_+$ and an AC^2 $\delta x : [0, T] \rightarrow \mathbb{R}^d$ such that $\delta x(0) = \delta x(T) = 0$ (observe that the variations are equal for both curves, which is the base of the *restriction*). With these elements, and assuming fixed endpoints $x(0), x(T), y(0), y(T)$, we can establish the restricted variational principle:

Theorem 4.1. *The equations*

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = -\mu J_-^{-(\alpha+\beta)} x, \quad (34a)$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{y}} \right) - \frac{\partial L}{\partial y} = -\mu J_+^{-(\alpha+\beta)} y, \quad (34b)$$

are sufficient conditions for the extremals of $\mathcal{S}(x, y)$ (32) under restricted calculus of variations (33).

It is important to remark that in the proof of this theorem (see [19]), it is crucial the use of the asymmetric integration by parts (13a) and the semigroup property (13b) of the fractional derivatives. In addition, it is also proven in [19, Proposition 3.2] that under even parity of L in the velocity variable, then (34b) reduces to (34a) in reversed time, i.e. $y(t) = x(T - t)$. Finally, it is easy to see that the dynamics (34), say the Lagrangian dynamics subject to fractional damping, reduces to the usual linear damped dynamics when $\alpha = \beta = 1/2$, according to (12).

In the following, we give several intermediary lemmas which are obtained by generalizing the results presented in

4.2. Discrete setting based on CQ. In [18], [19], the author applied the discretization procedure described in §2.2 and the Grünwald-Letnikov approximation for the fractional derivative to derive the so-called *fractional variational integrators*. In the following, we propose a generalization of this process using CQ. For that, let us consider two discrete series $x_d = \{x_k\}_{0:N}$ and $y_d = \{y_k\}_{0:N}$, as well as two particular discretizations of (11), i.e.

$$\mathcal{J}_-^{-\alpha} x_k = \sum_{n=0}^k \omega_n^{(-\alpha)} x_{k-n}, \quad \mathcal{J}_+^{-\beta} y_k = \sum_{n=0}^{N-k} \omega_n^{(-\beta)} y_{k+n}, \quad (35)$$

where the weights $\omega_n^{(-\alpha)}$ are the coefficients of the generating power series of $K^{(-\alpha)}(\gamma(z)/h)$ with $K^{(\alpha)}$ defined in (17), namely

$$K^{(-\alpha)} \left(\frac{\gamma(z)}{h} \right) = \left(\frac{\gamma(z)}{h} \right)^\alpha = \sum_{k=0}^{\infty} \omega_k^{(-\alpha)} z^k.$$

For concreteness, we choose again $\gamma_p(z)$ as in (30), the characteristic function of the backward differentiation formulas. The Grünwald weights used in [19] is equivalent to CQ with a particular choice of $\gamma_p(z)$, i.e. $\gamma_1(z) = 1 - z$ and the notation $\mathcal{J}_-^{-\alpha} x_k$ and $\mathcal{J}_+^{-\beta} y_k$ have been used as $\Delta_-^\alpha x_k$ and $\Delta_+^\beta y_k$ respectively.

The discrete action, counterpart of (32), is then

$$\begin{aligned}\mathcal{L}_d(x_d, y_d) &= \mathcal{S}_d^{\text{cons}}(x_d, y_d) + \mathcal{S}_d^{\text{frac}}(x_d, y_d), \\ \mathcal{S}_d^{\text{cons}}(x_d, y_d) &= \sum_{k=0}^{N-1} (L_d(x_k, x_{k+1}) + L_d(y_k, y_{k+1})), \quad \mathcal{S}_d^{\text{frac}}(x_d, y_d) = -\mu h \sum_{k=0}^N \mathcal{J}_-^{-\alpha} x_k \mathcal{J}_+^{-\beta} y_k.\end{aligned}\quad (36)$$

Taking the discrete equivalent of the restricted varied curves, i.e.

$$x_d^\epsilon = x_d + \epsilon \{\delta x_k\}_{0:N}, \quad y_d^\epsilon = y_d + \epsilon \{\delta y_k\}_{0:N}, \quad (37)$$

such that $\delta x_0 = \delta x_N = 0$, we can establish the discrete counterpart of Theorem (4.1):

Theorem 4.2. *The equations*

$$D_1 L_d(x_k, x_{k+1}) + D_2 L_d(x_{k-1}, x_k) = \mu h \mathcal{J}_-^{-(\alpha+\beta)} x_k, \quad (38a)$$

$$D_1 L_d(y_k, y_{k+1}) + D_2 L_d(y_{k-1}, y_k) = \mu h \mathcal{J}_+^{-(\alpha+\beta)} y_k, \quad (38b)$$

both for $k = 1, \dots, N-1$, are sufficient conditions for the extremals of $\mathcal{L}_d(x_d, y_d)$ (36) under restricted calculus of variations (37).

See [19] for the proof. As in the continuous side, the semigroup property and asymmetric integration by parts of the discrete fractional derivatives/integrals, properties (1) and (2) in Lemma 3.1, respectively, are crucial in the proof of this theorem. It is also true that (38b) reduces to (38a) in discrete reversed time, i.e. $y_k = x_{N-k}$ ([19], Proposition 4.2). Naturally, the equations (38) provide a discrete iteration scheme for the fractional damped dynamics (34), with $\gamma_1(z) = 1 - z$, delivering a $p = 1$ convergent integrator; see [19] for further details.

In the following section, we will apply the order two midpoint variational integrator for the conservative part [28] and BDFCQ for the fractional one. Then, we will denote by FVI-BDFCQ the scheme (38a) and write it simply FVI when no confusion can arise. All the experiments are carried out in Julia Version 1.9.3.

4.3. Numerical experiment. For the next example, we take the Lagrangian associated to the harmonic oscillator of the form $L(x, \dot{x}) = \dot{x}^2/2 - x^2/2$ so that the equation (34a) reads for $\alpha = \beta$

$$\ddot{x} + \mu D_-^{(2\alpha)} x + x = 0, \quad (39)$$

where $D_-^{(2\alpha)} \equiv J_-^{-(2\alpha)}$. Let us consider the problem on $[0, 16]$ and choosing $\alpha = 1/2$ so that fractional operator $D_-^{(2\alpha)}$ coincides with the usual operator d/dt . In this test run we take the initial values $x(0) = 0$, $\dot{x}(0) = 1.2$ and $\mu = 0.2$. Firstly we plot the numerical solution obtained by the FVI-BDF1CQ, explicit and implicit Euler integrators on the interval $[0, 16]$ with the stepsize $h = 0.125$ in Figure 3 (left). The corresponding results of the energy dissipation and the absolute errors are presented in Figure 3 (right) and Figure 4 (left), respectively. Secondly we compute the global errors as the maximum norm between the numerical solution and the exact solution, i.e.

$$\max |x(t_k) - x_k|, \quad \forall k.$$

The results are presented in Figure 4 (right) as the global errors (in logarithmic scale) against stepsizes on $[0, 16]$ with $h = 16/2^i$, $i = 4, \dots, 11$.

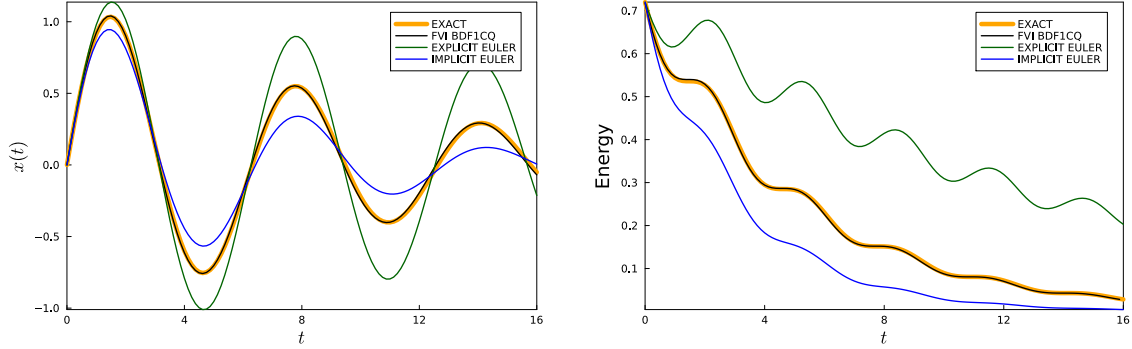


Figure 3. Damped harmonic oscillator (39) ($\alpha = 1/2$). Left: Exact solution vs FVI-BDF1CQ method for $h = 0.125$. Right: Energy behaviour for $h = 0.125$.

The main property of a dissipative system is that the energy is always dissipated with time and as we can see in Figure 3 (right), FVI-BDF1CQ can preserve the dissipation structure of the damped harmonic oscillator which confirm that FVI-BDF1CQ gives good numerical behaviour.

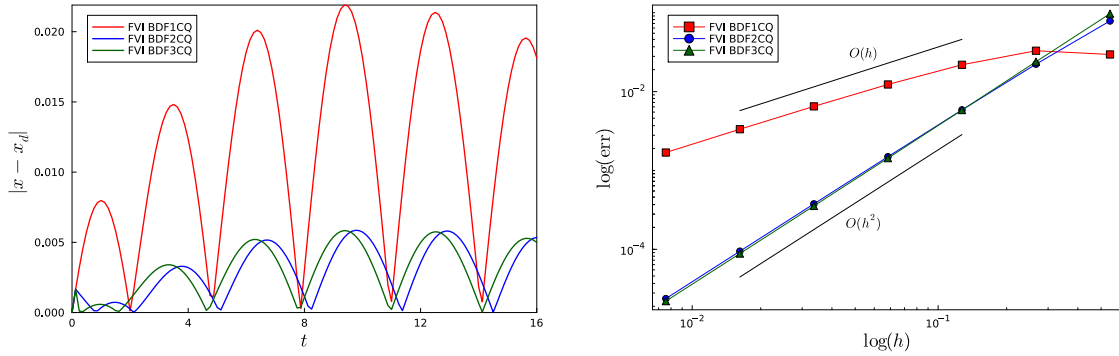


Figure 4. Damped harmonic oscillator (39). Left: absolute errors for $h = 0.125$. Right: Log-Log plot of the global error presented on $t \in [0, 16]$ for $h = 16/2^i$, $i = 4, \dots, 11$.

We can confirm from Figure 4 (right) that the order of FVI-BDF1CQ is one and this result has been discussed in [19]. However, we observe that the second order convergence both FVI-BDF2CQ and FVI-BDF3CQ which is natural since the midpoint integrator being used is of second order.

We also consider another example. Let us choose a Lagrangian of the forced harmonic oscillator problem defined by $L(t, x, \dot{x}) = \dot{x}^2/2 - x^2/2 + x f(t)$ with a non-vanishing function f . So that the equation (34a), again for $\alpha = \beta$, reads

$$\ddot{x} + \mu D_-^{(2\alpha)} x + x = f(t), \quad t \in [0, 1]. \quad (40)$$

For a non-integer 2α , this problem is known as Bagley-Torvik equation which can be used to describe, for example the dynamics of a rigid plate immersed in a Newtonian fluid when $\alpha = 3/4$ (see [34], [37]). Due to mathematical complexity, the analytic solutions of such equation are very few and are restricted to the one dimensional case. In particular, with the initial conditions $x(0) = \dot{x}(0) = 0$ and $\mu = 1$, the Bagley-Torvik equation is exactly solvable (see [13], [17]) by

considering,

$$f(t) = t^3 + 6t + \frac{3.2}{\Gamma(1/2)} t^2 \sqrt{t}, \quad \alpha = \frac{1}{4}, \quad (41a)$$

$$f(t) = \frac{15}{4} \sqrt{t} + \frac{15}{8} \sqrt{\pi} t + t^2 \sqrt{t}, \quad \alpha = \frac{3}{4}. \quad (41b)$$

where the analytic solutions are given, respectively, by $x(t) = t^3$ (resp. $= t^{\frac{5}{2}}$). We solve numerically the Bagley-Torvik problem (40) using FVI on $[0, 1]$ for $\alpha = \frac{1}{4}, \frac{3}{4}$. The global errors (in logarithmic scale) are presented in Figures 5 for $h = 1/2^i$, $i = 1, \dots, 8$.

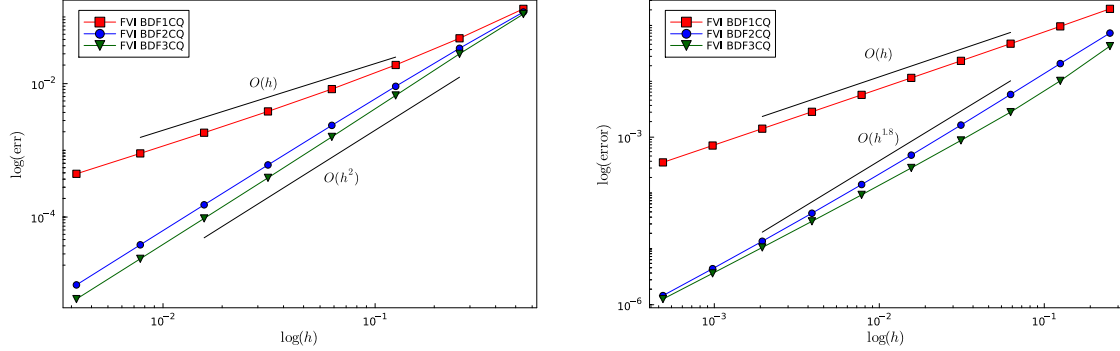


Figure 5. Bagley-Torvik equation (40). Log-Log plot of the global errors on $t \in [0, 1]$ for $h = 1/2^i$, $i = 1, \dots, 8$. Left: case (41a). Right: case (41b).

Again, it can be observed from Figure 5 that FVI-BDF1CQ leading to a convergence of order one. A convergence of order 2 for FVI-BDF2CQ and FVI-BDF3CQ is obtained (left plot) whereas a convergence of order cannot reach two for FVI-BDF2CQ and FVI-BDF3CQ (right plot).

We summarize the convergence order of (38a) for equations (39) and (40) in Table 1 where we consider the midpoint integrator for the conservative part.

	BDF1CQ	BDF2CQ	BDF3CQ
Damped oscillator ($\alpha = 1/2$)	order 1	order 2	order 2
Bagley-Torvik ($\alpha = 1/4$)	order 1	order 2	order 2
Bagley-Torvik ($\alpha = 3/4$)	order 1	order 1.8	order 1.8

Table 1. Convergence order of (38a) for equations (39) and (40).

5. HIGHER-ORDER FRACTIONAL VARIATIONAL INTEGRATORS BASED ON CONVOLUTION QUADRATURE

Now, we establish a particular discretization of the action (32), where we choose a higher-order approximation with quadrature rule $(b_i, c_i)_{i=1}^r$ (§2.3) for the conservative part $\mathcal{S}^{\text{cons}}$ and convolution quadrature (21), (22) for the fractional integrals involved in $\mathcal{S}^{\text{frac}}$ instead of the order 1 (35). For that, we take into account two discrete series $x_d = \{x_k\}_{0:N} \in (\mathbb{R}^d)^{N+1}$, $y_d = \{y_k\}_{0:N} \in (\mathbb{R}^d)^{N+1}$ and $s+1$ inner nodes $\{x_k^\nu\}^{0:s} \in (\mathbb{R}^d)^{s+1}$ in each interval $[k, k+1]$ such that $x_k^s = x_{k+1}^0$ (equiv. for

y). Namely

$$\begin{aligned} \mathcal{S}(x_d, y_d) &= \mathcal{S}_d^{\text{cons}}(x_d, y_d) + \mathcal{S}_d^{\text{frac}}(x_d, y_d), \\ \mathcal{S}_d^{\text{cons}}(x_d, y_d) &= \sum_{k=0}^{N-1} (L_d(x_k) + L_d(y_k)), \quad \mathcal{S}_d^{\text{frac}}(x_d, y_d) = -\mu h \sum_{k=0}^N \mathcal{J}_-^{-\alpha} x_k \mathcal{J}_+^{-\beta} y_k, \\ L_d(x_k) &= h \sum_{i=1}^r b_i L(x_d(c_i h; k), \dot{x}_d(c_i h; k)), \quad L_d(y_k) = h \sum_{i=1}^r b_i L(y_d(c_i h; k), \dot{y}_d(c_i h; k)), \end{aligned} \quad (42)$$

where the definition (6) applies for $x_d(t; k)$ and $y_d(t; k)$ just by $Q = \mathbb{R}^d$. Now, considering restricted varied curves

$$x_d^\epsilon = \{x_k^\nu\}_{0:N-1}^{0:s} + \epsilon \{\delta x_k^\nu\}_{0:N-1}^{0:s}, \quad y_d^\epsilon = \{y_k^\nu\}_{0:N-1}^{0:s} + \epsilon \{\delta y_k^\nu\}_{0:N-1}^{0:s}, \quad (43)$$

such that $\delta x_0 = \delta x_0^0 = 0$ and $\delta x_N = \delta x_{N-1}^s = 0$, we establish the following result (it is important to recall that, from now on, we shall consider the variation operator as $\delta \equiv d/d\epsilon|_{\epsilon=0}$, applied over the “varied” quantities). Before the theorem, we set a useful lemma.

Lemma 5.1. *According to the definitions (21), (22) and considering varied curves (43), we have that*

$$\delta \mathcal{J}_\lambda^{-\alpha} x_k = \mathcal{J}_\lambda^{-\alpha} \delta x_k.$$

Equivalently for y .

Proof. We pick $\sigma = -$, the proof for $+$ is equivalent. It is important to remark that in the convolution quadrature (21) the inner nodes are not involved, and consequently from (43) we only take into consideration the main nodes, i.e. $x_d^\epsilon = \{x_k\}_{0:N} + \epsilon \{\delta x_k\}_{0:N}$.

$$\delta \mathcal{J}_-^{-\alpha} x_k = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \mathcal{J}_-^{-\alpha} x_d^\epsilon = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} \sum_{n=0}^k \omega_n^{(-\alpha)} (x_{k-n} + \epsilon \delta x_{k-n}) = \sum_{n=0}^k \omega_n^{(-\alpha)} \delta x_{k-n} = \mathcal{J}_-^{-\alpha} \delta x_k.$$

□

Theorem 5.1. *The equations*

$$D_{s+1} L_d(x_{k-1}^0, \dots, x_{k-1}^s) + D_1 L_d(x_k^0, \dots, x_k^s) - \mu h \mathcal{J}_-^{-(\alpha+\beta)} x_k^0 = 0, \quad k = 1, \dots, N-1, \quad (44a)$$

$$D_i L_d(x_k^0, \dots, x_k^s) = 0, \quad k = 0, \dots, N-1, \quad i = 2, \dots, s, \quad (44b)$$

$$D_{s+1} L_d(y_{k-1}^0, \dots, y_{k-1}^s) + D_1 L_d(y_k^0, \dots, y_k^s) - \mu h \mathcal{J}_+^{-(\alpha+\beta)} y_k^0 = 0, \quad k = 1, \dots, N-1, \quad (44c)$$

$$D_i L_d(y_k^0, \dots, y_k^s) = 0, \quad k = 0, \dots, N-1, \quad i = 2, \dots, s, \quad (44d)$$

are sufficient conditions for the extremals of (42) under restricted calculus of variations (43).

Proof. From (42) we have that

$$\delta \mathcal{L}_d(x_d, y_d) = \delta \mathcal{S}_d^{\text{cons}}(x_d, y_d) + \delta \mathcal{S}_d^{\text{frac}}(x_d, y_d).$$

Let start to simplify $\delta \mathcal{S}_d^{\text{cons}}(x_d, y_d)$

$$\delta \mathcal{S}_d^{\text{cons}}(x_d, y_d) = \sum_{k=0}^{N-1} \left(\frac{\partial L_d(x_k)}{\partial x_k^\nu} + \frac{\partial L_d(y_k)}{\partial y_k^\nu} \right) \delta x_k^\nu,$$

where the summation over ν is understood and we have employed the restricted variations (43).

Concerning the term $\delta \mathcal{S}_d^{\text{frac}}(x_d, y_d)$ we have, let us use the notation

$$\frac{\partial L_d(x_k)}{\partial x_k^\nu} \delta x_k^\nu = D_i L_d(x_k) \delta x_k^{\nu_i}, \quad (45)$$

where on the left hand side $\nu = 0, \dots, s$ and on the right hand side $\nu_1 = 0, \nu_2 = 1, \dots, \nu_{s+1} = s$ (in other words $D_i = \partial/\partial x_k^{\nu_i}$); this way, it is highlighted that L_d is a function of $s+1$ variables (equiv. for y). Thus, we have

$$\begin{aligned} \delta \mathcal{S}_d^{\text{cons}}(x_d, y_d) &= \sum_{k=0}^{N-1} \sum_{i=1}^{s+1} (D_i L_d(x_k) + D_i L_d(y_k)) \delta x_k^{\nu_i}. \\ \delta \mathcal{S}_d^{\text{frac}}(x_d, y_d) &=^1 -\mu h \sum_{k=0}^N \mathcal{J}_-^{-\alpha} x_k \mathcal{J}_+^{-\beta} \delta x_k - \mu h \sum_{k=0}^N \mathcal{J}_-^{-\alpha} \delta x_k \mathcal{J}_+^{-\beta} y_k \\ &=^2 -\mu h \sum_{k=0}^N \mathcal{J}_-^{-\beta} \mathcal{J}_-^{-\alpha} x_k \delta x_k - \mu h \sum_{k=0}^N \delta x_k \mathcal{J}_+^{-\alpha} \mathcal{J}_+^{-\beta} y_k \\ &=^3 -\mu h \sum_{k=1}^{N-1} \left(\mathcal{J}_-^{-(\beta+\alpha)} x_k^0 + \mathcal{J}_+^{-(\alpha+\beta)} y_k^0 \right) \delta x_k^0. \end{aligned}$$

In $=^1$ we have employed the Leibnitz rule of the derivative and Lemma 5.1. In $=^2$ we have employed the asymmetric integration by parts, i.e. property (2) in Lemma 3.1. Finally, in $=^3$ we have rearranged terms, employed the semigroup property (1) in Lemma 3.1, taken into account that $x_k = x_k^0$, $y_k = y_k^0$ and $\delta x_k = \delta x_k^0$ in terms of the inner nodes and taken also into account that $\delta x_0 = \delta x_N = 0$, such that the terms $k=0$ and $k=N$ vanish.

Putting everything together we have

$$\begin{aligned} \delta \mathcal{L}_d(x_d, y_d) &= \sum_{k=0}^{N-1} \sum_{i=1}^{s+1} (D_i L_d(x_k) + D_i L_d(y_k)) \delta x_k^{\nu_i} - \mu h \sum_{k=1}^{N-1} \left(\mathcal{J}_-^{-(\alpha+\beta)} x_k^0 + \mathcal{J}_+^{-(\alpha+\beta)} y_k^0 \right) \delta x_k^0 \\ &= \sum_{k=0}^{N-1} \sum_{i=2}^{s+1} D_i L_d(x_k) \delta x_k^{\nu_i} + \sum_{k=1}^{N-1} \left(D_1 L_d(x_k) - \mu h \mathcal{J}_-^{-(\alpha+\beta)} x_k^0 \right) \delta x_k^0 \\ &\quad + \sum_{k=0}^{N-1} \sum_{i=2}^{s+1} D_i L_d(y_k) \delta x_k^{\nu_i} + \sum_{k=1}^{N-1} \left(D_1 L_d(y_k) - \mu h \mathcal{J}_+^{-(\alpha+\beta)} y_k^0 \right) \delta x_k^0 \end{aligned}$$

where is taken into account that $\delta x_0 = \delta x_N = 0$ and that $D_{s+1} L_d(x_{k-1}) = D_1 L_d(x_k)$. Now, given that $\delta x_k^{\nu_i}$ are arbitrary for $k = 0, \dots, N-1$, $i = 1, \dots, s+1$ (except δx_0), we see from the last equality that

$$\begin{aligned} D_i L_d(x_k) &= 0, & k &= 0, \dots, N-1, \quad i = 2, \dots, s, \\ D_{s+1} L_d(x_{k-1}) + D_1 L_d(x_k) - \mu h \mathcal{J}_-^{-(\alpha+\beta)} x_k^0 &= 0, & k &= 1, \dots, N-1, \\ D_i L_d(y_k) &= 0, & k &= 0, \dots, N-1, \quad i = 2, \dots, s, \\ D_{s+1} L_d(y_{k-1}) + D_1 L_d(y_k) - \mu h \mathcal{J}_+^{-(\alpha+\beta)} y_k^0 &= 0, & k &= 1, \dots, N-1, \end{aligned}$$

is a sufficient condition for $\delta \mathcal{L}_d(x_d, y_d) = 0$ and the claim holds. \square

Remark 5.1. The partial derivatives of $L_d(x_k)$ (equiv. y) are completely determined by the quadrature rule $(b_i, c_i)_{i=1}^r$ and the Lagrangian function $L(q, \dot{q})$, according to (42) and (6). Namely

$$\begin{aligned} \frac{\partial L_d(x_k)}{\partial x_k^{\nu}} &= h \sum_{i=1}^r b_i \left(\frac{\partial L}{\partial q}(x_d(c_i h; k), \dot{x}_d(c_i h; k)) \frac{\partial x_d}{\partial x_k^{\nu}} + \frac{\partial L}{\partial \dot{q}}(x_d(c_i h; k), \dot{x}_d(c_i h; k)) \frac{\partial \dot{x}_d}{\partial x_k^{\nu}} \right) \\ &= h \sum_{i=1}^r b_i \left(\frac{\partial L}{\partial q}(x_d(c_i h; k), \dot{x}_d(c_i h; k)) \ell_{\nu}(c_i h) + \frac{\partial L}{\partial \dot{q}}(x_d(c_i h; k), \dot{x}_d(c_i h; k)) \frac{1}{h} \ell_{\nu}(c_i h) \right). \end{aligned}$$

Naturally, equations (44a),(44b) can be employed as a discrete iteration scheme for the dynamics (34a), the same way (44c),(44d) can be used for (34b). We shall focus on the x -part, since y is equivalent.

The equations

$$\begin{aligned} p_{x_0} &:= -D_1 L_d(x_0^0, \dots, x_0^s), \\ 0 &= D_i L_d(x_k^0, \dots, x_k^s), \quad \forall i = 2, \dots, s, \quad k = 0, \dots, N-1, \\ 0 &= D_{s+1} L_d(x_{k-1}^0, \dots, x_{k-1}^s) + D_1 L_d(x_k^0, \dots, x_k^s) - \mu h \mathcal{J}_-^{-(\alpha+\beta)} x_k^0, \quad k = 1, \dots, N-1, \end{aligned}$$

(where we include the initial momentum $p_{x_0} := -D_1 L_d(x_0^0, \dots, x_0^s)$ as a definition ⁸) conform a discrete iteration scheme

$$\begin{aligned} x_0^0 &\mapsto (x_0^0, \dots, x_0^s = x_1^0), \\ (x_{k-1}^0, \dots, x_{k-1}^s = x_k^0) &\mapsto (x_k^0, \dots, x_k^s = x_{k+1}^0), \quad k = 1, \dots, N-1, \end{aligned}$$

that can be represented as an algorithm:

Algorithm 1 Higher-order fractional variational integrator (with convolution quadrature)

- 1: **Initial data:** $N, h, \alpha, \beta, \omega_n^{-(\alpha+\beta)}, \mu, x_0^0, p_{x_0}$.
- 2: **solve for** x_0^1, \dots, x_0^s **from**

$$\begin{aligned} p_{x_0} &= -D_1 L_d(x_0^0, \dots, x_0^s), \\ 0 &= D_i L_d(x_0^0, \dots, x_0^s), \quad \forall i = 2, \dots, s. \end{aligned}$$

- 3: **Initial points:** $x_0^0, \dots, x_0^s = x_1^0$
- 4: **for** $k = 1 : N-1$ **do**
 solve for $x_k^1, \dots, x_k^s = x_{k+1}^0$ **from**

$$\begin{aligned} 0 &= D_{s+1} L_d(x_{k-1}^0, \dots, x_{k-1}^s) + D_1 L_d(x_k^0, \dots, x_k^s) - \mu h \sum_{n=0}^k \omega_n^{-(\alpha+\beta)} x_{k-n}^0, \\ 0 &= D_i L_d(x_k^0, \dots, x_k^s), \quad \forall i = 2, \dots, s. \end{aligned}$$

- 5: **end for**
 - 6: **Output:** $(x_1^\nu, \dots, x_{N-1}^\nu), \quad \nu = 0, \dots, s$.
-

It is important to remark that at each step a nonlinear system of s algebraic equations is solved in order to obtain the s unknowns $(x_k^1, \dots, x_k^s = x_{k+1}^0)$, even in the initialization step.

5.1. Numerical experiment. We will employ a variational integrators of order 4 for the conservative part based on two points Gauss quadrature and a polynomial degree 2 (see [31]) and BDFCQ for the fractional one. To simplify notation, we continue to write FVI-BDFCQ (or only FVI when it is convenient) for equations 44a and 44b and the numerical solution can be computed using Algorithm 1.

Let us consider the previous examples as in §4.3. As expected, we notice in Figures 6 and 7 that FVI-BDF1CQ and FVI-BDF2CQ are of first and second order, respectively. From the numerical point of view one would expect a higher accuracy (order 3 using BDF3CQ mixed with third order variational integrator) which we do not get. One possible reason might be mixing of integrators (VI and BDFCQ). In particular, BDFCQ depends only the main nodes but not on the inner nodes which are considered in the conservative part. Another possible reason might be saturation effects coming from CQ as described in §3.3.

⁸Naturally, this definition is based on the Hamiltonian version of discrete mechanics, which can be consulted for conservative systems in [28], and for the particular case of fractional damping in [19]. We do not enter here in further details since it is offtopic.

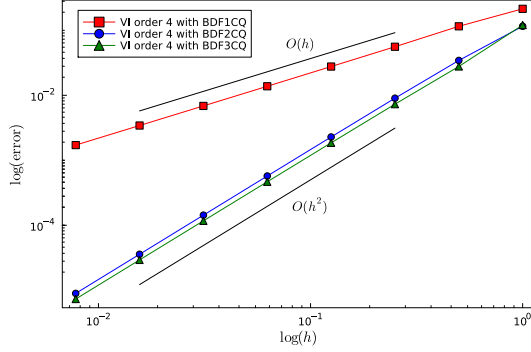


Figure 6. Damped harmonic oscillator (39). Log-Log plot of the global error presented on $t \in [0, 16]$ for $h = 16/2^i$, $i = 4, \dots, 11$.

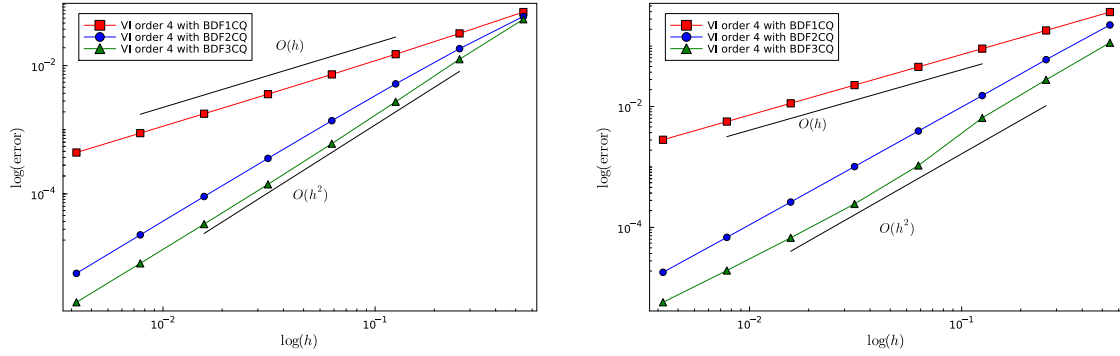


Figure 7. Bagley-Torvik equation (40). Log-Log plot of the global error on $t \in [0, 1]$ for $h = 1/2^i$, $i = 1, \dots, 8$. Left: case (41a). Right: case (41b).

As we have seen in §3.3, the main issue of using BDFCQ for certain class of solution functions is that one cannot achieve a high accuracy, see the saturation effects in Figures 2. However, a correction term should be added as in (26) to recover the order of accuracy as the one of the underlying BDF methods. We apply BDF3CQ with a correction term in Algorithm 1 for equation (40) when $\alpha = 3/4$ and as we observe in Figure 8, the third order accuracy is almost achieved. However, this phenomenon does not work with the previous studied cases which seems related to the accumulation of errors.

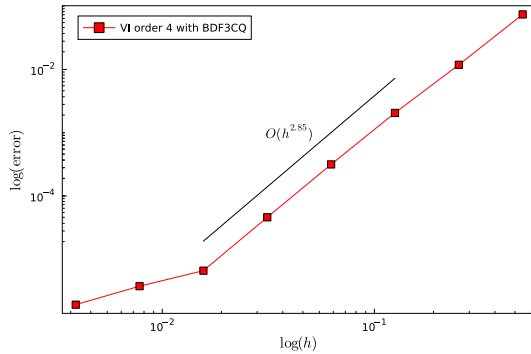


Figure 8. Bagley-Torvik equation (40), case (41b), i.e. $\alpha = 3/4$. Log-Log plot of the global error on $t \in [0, 1]$ for $h = 1/2^i$, $i = 1, \dots, 8$.

We summarize the convergence order of (38a) for equations (39) and (40) in Table 2 where we consider an integrator of order 4 for the conservative part.

	BDF1CQ	BDF2CQ	BDF3CQ
Damped oscillator ($\alpha = 1/2$)	order 1	order 2	order 2
Bagley-Torvik ($\alpha = 1/4$)	order 1	order 2	order 2
Bagley-Torvik ($\alpha = 3/4$)	order 1	order 2	order 2

Table 2. Convergence order of (38a) for equations (39) and (40).

6. CONCLUSIONS

A restricted Hamilton's principle is a new class of fractional calculus of variations has been introduced in [18], [19]. The main motivation of this approach is to derive the dynamics of fractionally damped systems (1) using a purely variational way and hence to construct the so-called fractional variational integrators (FVIs).

We have developed FVIs that combine the convolution quadrature (CQ), which is particularly suitable [24], [26] in the framework of the restricted Hamilton's principle, with the variational integrators [16], [28], [31]. Our result coincides, in particular, with the one given in [19] when using the classical variational integrators.

This work centers around increasing the accuracy the numerical scheme associated to (1). Here, we have focused on implementing the FVIs and test numerically their accuracy using two mechanical systems, the damped harmonic oscillator and the Bagley-Torvik problems. We notice that for FVI based on BDFCQ, it can only achieve the second-order accuracy even for a higher-order FVI (see Figures 6 and 7) which is due to the fact that saturation effects are also a part of the problem. In this situation, with the use of correction term, the third-order accuracy for FVI-BDF3CQ is observed in Figure (8).

To overcome the problem of limitation with this strategy i.e. in order to obtain the same order of convergence of the underlying BDF methods, it will be necessary to take a correction term in to account which is difficult, in general, to deal with for some values of α and further errors are arising from solving the linear systems of the starting quadrature [12].

Another problem of using BDFCQ is that, the inner nodes used in a higher-order approximation for the conservative action (32) are not taken into account in BDFCQ for the fractional one. Thus, a way to handle this is to apply the high-order Runge-Kutta convolution quadrature (RKCQ) [4], [27] for the fractional part which will be a future work.

REFERENCES

- [1] R. ABRAHAM and J. E. MARSDEN, *Foundations of Mechanics*. Benjamin/Cummings Publishing Company, (1978).
- [2] O. P. AGRAWAL, “Formulation of Euler–Lagrange equations for fractional variational problems,” *Journal of Mathematical Analysis and Applications* **272**(1), pp. 368–379, (2002).
- [3] H. M. S. ANATOLY A. KILBAS and J. J. TRUJILLO, *Theory and Applications of Fractional Differential Equations*, North-Holland Mathematics Studies 204, 1st ed. Elsevier, (2006).
- [4] L. BANJAI and C. LUBICH, “RAn error analysis of Runge–Kutta convolution quadrature,” *BIT Numerical Mathematics* **51**(3), pp. 483–496, (2011).
- [5] H. BATEMAN, “On dissipative systems and related variational principles,” *Phys. Rev.* **38**, pp. 815–819, (1931).
- [6] L. BOURDIN, J. CRESSON, I. GREFF, and P. INIZAN, “Variational integrator for fractional Euler–Lagrange equations,” *Applied Numerical Mathematics* **71**, pp. 14–23, (2013).
- [7] C. M. CAMPOS, “High order variational integrators: A polynomial approach,” in *Advances in Differential Equations and Applications*, F. CASAS and V. MARTÍNEZ, Eds. Springer International Publishing, (2014), vol. 4, pp. 249–258.
- [8] C. M. CAMPOS, S. OBER-BLÖBAUM, and E. TRÉLAT, “High order variational integrators in the optimal control of mechanical systems,” *Discrete and Continuous Dynamical Systems* **35**(9), pp. 4193–4223, (2015).
- [9] J. CRESSON and P. INIZAN, “Variational formulations of differential equations and asymmetric fractional embedding,” *Journal of Mathematical Analysis and Applications* **385**(2), pp. 975–997, (2012).
- [10] D. M. DE DIEGO and R. S. M. DE ALMAGRO, “Variational order for forced lagrangian systems,” *Nonlinearity* **31**(8), p. 3814, (2018).
- [11] K. DIETHELM, *The Analysis of Fractional Differential Equations: An Application-Oriented Exposition Using Differential Operators of Caputo Type*, Lecture Notes in Mathematics 2004, 1st ed. Springer-Verlag Berlin Heidelberg, (2010).
- [12] K. DIETHELM, J. M. FORD, N. J. FORD, and M. WEILBEER, “Pitfalls in fast numerical solvers for fractional differential equations,” *Journal of Computational and Applied Mathematics* **186**(2), pp. 482–503, (2006).
- [13] N. J. FORD and J. A. CONNOLLY, “Systems-based decomposition schemes for the approximate solution of multi-term fractional differential equations,” *Journal of Computational and Applied Mathematics* **229**(2), pp. 382–391, (2009).
- [14] C. R. GALLEY, “Classical mechanics of nonconservative systems,” *Phys. Rev. Lett.* **110**, p. 174301, (2013).
- [15] E. HAIRER, C. LUBICH, and G. WANNER, *Geometric numerical integration*, Springer Series in Computational Mathematics, Second. Springer-Verlag, Berlin, (2006), **31**, pp. xviii+644, Structure-preserving algorithms for ordinary differential equations, ISBN: 3-540-30663-3; 978-3-540-30663-4.
- [16] J. HALL and M. LEOK, “Spectral variational integrators,” *Numerische Mathematik* **130**(4), pp. 681–740, (2015).
- [17] R. M. JENA and S. CHAKRAVERTY, “Analytical solution of Bagley–Torvik equations using Sumudu transformation method,” *SN Applied Sciences* **1**, p. 246, (2019).
- [18] F. JIMÉNEZ and S. OBER-BLÖBAUM, “A fractional variational approach for modelling dissipative mechanical systems: continuous and discrete settings,” *IFAC-PapersOnLine* **51**(3), pp. 50–55, (2018).
- [19] F. JIMÉNEZ and S. OBER-BLÖBAUM, “Fractional damping through restricted calculus of variations,” *Journal of Nonlinear Science* **31**, p. 46, (2021).
- [20] M. LEOK and T. SHINGEL, “General techniques for constructing variational integrators,” *Frontiers of Mathematics in China* **7**(2), pp. 273–303, (2012).
- [21] J. L. LOVOIE, T. J. OSLER, and R. TREMBLAY, “Fractional derivatives and special functions,” *SIAM Review* **18**(2), pp. 240–268, (1976).

- [22] C. LUBICH, “Fractional linear multistep methods for Abel–Volterra integral equations of the second kind,” *Math. Comp.* **45**, pp. 463–469, (1985).
- [23] C. LUBICH, “A stability analysis of convolution quadratures for Abel–Volterra integral equations,” *IMA J. Numer. Anal.* **6**, pp. 87–101, (1986).
- [24] C. LUBICH, “Convolution quadrature and discretized operational calculus. I and II,” *Numerische Mathematik* **52**, 129–145 and 413–425, (1988).
- [25] C. LUBICH, “On the multistep time discretization of linear initial-boundary value problems and their boundary integral equations,” *Numerische Mathematik* **67**, pp. 365–389, (1994).
- [26] C. LUBICH, “Discretized fractional calculus,” *SIAM Journal on Mathematical Analysis* **17**(3), pp. 704–719, (1986).
- [27] C. LUBICH and A. OSTERMANN, “Runge–Kutta methods for parabolic equations and convolution quadrature,” *Mathematics of Computation* **60**(201), pp. 105–131, (1993).
- [28] J. E. MARSDEN and M. WEST, “Discrete mechanics and variational integrators,” *Acta Numerica* **10**, pp. 357–514, (2001).
- [29] J. MOSER and A. P. VESELOV, “Galerkin variational integrators and modified symplectic Runge–Kutta methods,” *IMA Journal of Numerical Analysis* **139**, pp. 217–243, (1991).
- [30] S. OBER-BLÖBAUM, “Galerkin variational integrators and modified symplectic Runge–Kutta methods,” *IMA Journal of Numerical Analysis* **37**(1), pp. 375–406, (2016).
- [31] S. OBER-BLÖBAUM and N. SAAKE, “Construction and analysis of higher order galerkin variational integrators,” *Advances in Computational Mathematics* **41**, pp. 955–986, (2015).
- [32] S. OBER-BLÖBAUM and M. VERMEEREN, “Superconvergence of galerkin variational integrators,” *IFAC-PapersOnLine* **54**(19), pp. 327–333, (2021).
- [33] K. B. OLDHAM and J. SPANIER, *The fractional calculus: Theory and Applications of Differentiation and Integration to Arbitrary Order*. Academic Press, New York, London, (1974).
- [34] I. PODLUBNY, *Fractional Differential Equations: An Introduction to Fractional Derivatives, Fractional Differential Equations, to Methods of Their Solution and Some of Their Applications*, Mathematics in Science and Engineering **198**, 1st. Academic Press, (1998).
- [35] F. RIEWE, “Nonconservative lagrangian and hamiltonian mechanics,” *Phys. Rev. E* **53**(2), pp. 1890–1899, (1996).
- [36] S. G. SAMKO, A. A. KILBAS, and O. I. MARICHEV, *Fractional Integrals and Derivatives: Theory and Applications*, 1st ed. Gordon, (1993).
- [37] P. J. TORVIK and R. L. BAGLEY, “On the appearance of the fractional derivative in the behavior of real materials,” *Journal of Applied Mechanics* **51**(2), pp. 294–298, (1984).

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