Abstract. — In this paper, we introduce the notion of discrete embedding which is an algebraic procedure associating a numerical scheme to a given ordinary differential equation. We first define the Gauss finite differences embedding. In this setting, we study variational integrator on classical Lagrangian systems. Finally, we extend these constructions to the fractional case. In particular, we define the Gauss Grünwald-Letnikov embedding and the corresponding variational integrator on fractional Lagrangian systems.

Keywords: Lagrangian systems, Variational integrator, Fractional calculus.

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Introduction

Fractional calculus is a source of many investigations for the purposes of Physics and Engineering (see [4], [15], [18], [22], [24]). For example, fractional terms appear numerically in the modeling of the flow of a fluid in a heterogeneous environment, [25]. In Mathematics, we find fractional calculus in the probability theory, [20]. Moreover, due to their nonlocal characteristic and consequently due to their capacity of memory, fractional differential operators are also interesting for financial mathematics, [10], and for modeling of some materials like gum and rubber.

In recent years, many studies have been devoted to fractional Lagrangian systems, [11]. They arise for example in fractional optimal control theory ([1], [2], [14], [16]) and they are difficult to solve explicitly (see [22] for a general study). Then, it is interesting to develop efficient numerical schemes to such systems.

There exists a suitable method for classical Lagrangian systems called variational integrators which is developed in [17], [21]. Indeed, classical Lagrangian systems possess a variational structure, i.e. their solutions correspond to critical points of a functional and this characterization does not depend on the coordinates system, [5]. This structure induces strong constraints on the qualitative behavior of the solutions, as for example the conservation of energy for autonomous classical Lagrangian systems.

The basic idea of a variational integrator is to preserve this variational structure at the discrete level. We can obtain this numerical scheme by forming a discrete analogous of the variational principle on a discrete version of the Lagrangian functional.

Following the usual strategy of [17] and [21], this paper is devoted to the extension of variational integrators to the fractional case in the framework of discrete embeddings.

More precisely, we first define the notion of discrete embedding which gives a direct discrete analogous of a given differential equation (in particular of a given Lagrangian system). This procedure is algebraic and mainly based on the form of differential operators which is coordinates dependent. Consequently, this process does not necessary conserve at the discrete level the intrinsic Lagrangian structure of a Lagrangian system.

On the other hand, a discrete embedding gives a discrete version of a given Lagrangian functional and we can develop a discrete calculus of variations on this one which leads to a variational integrator of the associated Lagrangian system.

Then, by defining a discrete embedding, we obtain two discretizations of a Lagrangian system: the direct one and the variational integrator. Of course, these two discretizations are not necessary the same: in this case, we say that the discrete embedding is not coherent.

In this paper, we first prove that the basic finite differences discrete embedding is not coherent in the classical case. However, this default of coherence can be corrected by
rewriting, with left and right derivatives, the classical differential equation of Lagrangian systems. Indeed, this asymmetric rewriting corresponds at the continuous level to the discrete version of Lagrangian systems obtained by variational integrator. As a consequence, the discrete embedding is coherent in the asymmetric case.

In the fractional case, the derivatives are naturally asymmetric and satisfy a fractional integration by parts. In this paper, we prove that the fractional Grünwald-Letnikov discrete embedding is coherent.

The discretization of fractional Euler-Lagrange equations has been discussed by several authors. We refer in particular to [3] for finite element methods to fractional Lagrangian functionals, to [7] and [8] for a discrete fractional calculus of variations and to [6] for a numerical scheme on fractional optimal control problems. Some preliminary results on fractional discrete operators have already been discussed in these papers.

However, the discrete embedding point of view and the associated notion of variational integrator are not introduced in these papers as well as the corresponding coherence problem.

The paper is organized as follows. In section [1], we define the notion of discrete embeddings and direct discrete embeddings of a differential equation. Section [2] recalls definitions and results concerning Lagrangian systems. Then, we apply the previous theory of discrete embeddings to Lagrangian systems. Section [3] recalls the strategy of variational integrators in the framework of discrete embeddings. Noticing a default of coherence of the previous discrete embedding, we define in section [4] asymmetric derivatives and then asymmetric Lagrangian systems. With these asymmetric notations, we correct the default of coherence. Section [5] is an introduction to fractional calculus. Finally, section [6] is devoted to fractional discrete embeddings and the associated fractional variational integrators.

1. Notion of discrete embeddings

In this paper, we consider classical and fractional differential systems in $\mathbb{R}^d$ where $d \in \mathbb{N}^*$ is the dimension. The trajectories of these systems are curves $q \in C^0([a, b], \mathbb{R}^d)$ where $a < b$ are two reals. For smooth enough functions $q$, we denote $\dot{q} = \frac{dq}{dt}$ and $\ddot{q} = \frac{d^2q}{dt^2}$.

1.1. Discrete embeddings. — A discrete embedding is a particular way to give a discrete analogous of an ordinary differential equation:

**Definition 1.** — *Defining a discrete embedding* means giving a discrete version of the following elements: the curves $q \in C^0([a, b], \mathbb{R}^d)$, the derivative operator $\frac{d}{dt}$ and the functionals $a : C^0([a, b], \mathbb{R}^d) \rightarrow \mathbb{R}$. More precisely, it means giving:

- an application $q \mapsto q^h$ where $q^h \in (\mathbb{R}^d)^{m_1}$,
- a discrete operator $\Delta : (\mathbb{R}^d)^{m_1} \rightarrow (\mathbb{R}^d)^{m_2}$ which discretizes the differential operator $\frac{d}{dt}$.
- an application $a \mapsto a^h$ where $a^h : (\mathbb{R}^d)^{m_1} \rightarrow \mathbb{R}$, where $m_1, m_2 \in \mathbb{N}^*$.

Obviously, the discretization of curves above-defined induces the discrete evaluation of a function $f \in C^0(\mathbb{R}^d, \mathbb{R}^m)$, $m \in \mathbb{N}^*$ on the curves $q$. Indeed, by abusing the notation, if we denote by $f$ the following application
\[
f : \ C^0([a, b], \mathbb{R}^d) \rightarrow C^0([a, b], \mathbb{R}^m) \ , \quad q \mapsto f \circ q\]
then the discretization of $f$ is $f^h$ given by:
\[
f^h : (\mathbb{R}^d)^{m_1} \rightarrow (\mathbb{R}^m)^{m_1} \quad q^h \mapsto f^h(q^h) := \left(f(q^h_k)\right)_{k=1,...,m_1}.
\]

However, the discretization of a functional is not obvious. Indeed, it could use the discretization of $\frac{d}{dt}$ and the discretization of other mathematical tools depending on the form of the functional itself. We are giving an example in subsection 3.1 with the discretization of a Lagrangian functional is written with an integral.

In order to illustrate definition 1, we define forward and backward finite differences embedding. For all the rest of the paper, we fix $\sigma = \pm$ and $N \in \mathbb{N}^*$. We denote by $h = \frac{b - a}{N}$ the step size of the discretization and $\tau = (t_k)_{k=0,...,N}$ the following partition of $[a, b]$:
\[
\forall k \in \{0,...,N\}, \ t_k = a + k \frac{b - a}{N}.
\]
Now, we can define the following discrete embeddings:

**Definition 2 (case $\sigma = +$).** — We call forward finite differences embedding denoted by $\text{FDE}^+$ the definition of the following elements: the application
\[
disc : \ C^0([a, b], \mathbb{R}^d) \rightarrow (\mathbb{R}^d)^{N+1} \quad q \mapsto (q(t_k))_{k=0,...,N}
\]
and the discrete operator
\[
\Delta^+ : (\mathbb{R}^d)^{N+1} \rightarrow (\mathbb{R}^d)^N \quad Q = (Q_k)_{k=0,...,N} \mapsto \left(\frac{Q_k - Q_{k+1}}{h}\right)_{k=0,...,N-1}.
\]

**Definition 3 (case $\sigma = -$).** — We call backward finite differences embedding denoted by $\text{FDE}^-$ the definition of the following elements: the application
\[
disc : \ C^0([a, b], \mathbb{R}^d) \rightarrow (\mathbb{R}^d)^{N+1} \quad q \mapsto (q(t_k))_{k=0,...,N}
\]
and the discrete operator
\[
\Delta^- : (\mathbb{R}^d)^{N+1} \rightarrow (\mathbb{R}^d)^N \quad Q = (Q_k)_{k=0,...,N} \mapsto \left(\frac{Q_{k-1} - Q_k}{h}\right)_{k=1,...,N}.
\]
and the discrete operator
\[
\Delta_\sigma : \quad (\mathbb{R}^d)^{N+1} \rightarrow (\mathbb{R}^d)^N \quad Q = (Q_k)_{k=0,\ldots,N} \mapsto \left( \frac{Q_k - Q_{k-1}}{h} \right)_{k=1,\ldots,N}
\]

We use these notations in order to be uniform with fractional notations (in sections 5-6).

Let us notice that the discrete analogous of \( \frac{d}{dt} \) in \( FDE_{\sigma} \) is then \( -\sigma \Delta_{\sigma} \).

1.2. Direct discrete embedding. — Defining a discrete embedding allows us to define a direct discrete version of a differential equation:

**Definition 4.** — Let be fixed a discrete embedding defined as in definition [7] and let \((\mathcal{E})\) be an ordinary differential equation of unknown \( q \in \mathcal{C}^0([a,b],\mathbb{R}^d) \) given by:

\[
(\mathcal{E}) \quad O(q) = 0
\]

where \( O \) is a differential operator shaped as \( O = \sum_i f_i(\cdot) \frac{d}{dt} g_i(\cdot) \) where \( f_i, g_i \) are functions.

Then, the **direct discrete embedding** of \((\mathcal{E})\) is \((\mathcal{E}_h)\) the system of equations of unknown \( q^h \in (\mathbb{R}^d)^m \) given by:

\[
(\mathcal{E}_h) \quad O^h(q^h) = 0
\]

where \( O^h \) is the discretized operator of \( O \) given by \( O^h = \sum_i f^h_i(\cdot) \Delta \circ g^h_i(\cdot) \).

**Example 1.** — We consider the Newton’s equation with friction of unknown \( q \in \mathcal{C}^0([a,b],\mathbb{R}^d) \) given by:

\[
(NE) \quad \forall t \in [a,b], \quad \ddot{q}(t) + \dot{q}(t) + q(t) = 0.
\]

Then, the direct discrete embedding of \((NE)\) with respect to \( FDE_{\cdot} \) is \((NE_h)\) the system of equations of unknown \( Q \in (\mathbb{R}^d)^{N+1} \) given by:

\[
(NE_h) \quad \forall k \in \{0,\ldots,N-2\}, \quad \frac{Q_{k+2} - 2Q_{k+1} + Q_k}{h^2} + \frac{Q_{k+1} - Q_k}{h} + Q_k = 0.
\]

The direct discrete embedding of an ordinary differential equation is strongly dependent on the form of the differential operator \( O \) (and not on its equivalence class). The process \( O \rightarrow O^h \) is not an application. For example, the discretized operator \( O^h \) of \( O = \frac{d}{dt} \circ \sin(\cdot) = \frac{d}{dt}(\cdot) \cos(\cdot) \) is different depending on the writing of \( O \).

2. Discrete embeddings of Lagrangian systems

2.1. Lagrangian systems. — In this section, we recall classical definitions and theorems concerning Lagrangian systems. We refer to [5] for a detailed study and for the proof of theorem [1].
Definition 5. — A Lagrangian functional is an application defined by:

\begin{equation}
\mathcal{L} : \mathcal{C}^2([a,b], \mathbb{R}^d) \rightarrow \mathbb{R}
\end{equation}

\[ q \mapsto \int_a^b L(q(t), \dot{q}(t), t) \, dt \]

where \( L \) is a Lagrangian i.e. a \( \mathcal{C}^2 \) application defined by:

\[ L : \mathbb{R}^d \times \mathbb{R}^d \times [a,b] \rightarrow \mathbb{R} \]

\[ (x,v,t) \mapsto L(x,v,t) \].

Let \( L \) be a Lagrangian functional, we denote by \( D\mathcal{L}(q)(w) \) the Fréchet derivative of \( \mathcal{L} \) in \( q \) along the direction \( w \) in \( \mathcal{C}^2([a,b], \mathbb{R}^d) \), i.e.

\[ D\mathcal{L}(q)(w) = \lim_{\varepsilon \to 0} \frac{\mathcal{L}(q + \varepsilon w) - \mathcal{L}(q)}{\varepsilon} \].

An extremal (or critical point) of a Lagrangian functional \( \mathcal{L} \) is a trajectory \( q \) such that \( D\mathcal{L}(q)(w) = 0 \) for any variations \( w \) (i.e. \( w \in \mathcal{C}^2([a,b], \mathbb{R}^d) \), \( w(a) = w(b) = 0 \)).

Extremals of a Lagrangian functional can be characterized as solution of a differential equation of order 2 given by:

**Theorem 1 (Variational principle).** — Let \( \mathcal{L} \) be a Lagrangian functional associated to the Lagrangian \( L \) and let \( q \in \mathcal{C}^2([a,b], \mathbb{R}^d) \). Then, \( q \) is an extremal of \( \mathcal{L} \) if and only if \( q \) is solution of the Euler-Lagrange equation given by:

\[ \forall t \in [a,b], \quad \frac{\partial L}{\partial x}(q(t), \dot{q}(t), t) - \frac{d}{dt} \left( \frac{\partial L}{\partial v}(q(t), \dot{q}(t), t) \right) = 0. \]

2.2. Direct discrete embedding of the Euler-Lagrange equation. — In this subsection, we apply definitions of section I in order to define the direct discrete embedded Euler-Lagrange equation.

Definition 6. — Let \( L \) be a Lagrangian and \( \mathbf{[EL]} \) its associated Euler-Lagrange equation. The direct discrete embedding of \( \mathbf{[EL]} \) with respect to \( \text{FDE}_\sigma \) is given by:

\begin{equation}
\frac{\partial L}{\partial x}(Q, -\sigma \Delta_\sigma Q, \tau) + \sigma \Delta_\sigma \left( \frac{\partial L}{\partial v}(Q, -\sigma \Delta_\sigma Q, \tau) \right) = 0, \quad Q \in (\mathbb{R}^d)^{N+1}.
\end{equation}

We illustrate this result with the classical example of the mechanical Lagrangian:

\[ L(x,v,t) = \frac{1}{2} v^2 - U(x), \quad (x,v,t) \in \mathbb{R}^d \times \mathbb{R}^d \times [a,b] \]

where \( U \) represents the potential energy of the system. The mechanical Lagrangian gives the following Euler-Lagrange equation:

\[ \forall t \in [a,b], \quad \ddot{q}(t) = -\nabla U(q(t)), \quad q \in \mathcal{C}^2([a,b], \mathbb{R}^d). \]

Then, by direct discrete embedding with respect to \( \text{FDE}_- \), we obtain the following numerical scheme:

\[ \forall k \in 2, ..., N, \quad \frac{Q_k - 2Q_{k-1} + Q_{k-2}}{h^2} = -\nabla U(Q_k), \quad Q \in (\mathbb{R}^d)^{N+1}. \]
3. Discrete embeddings and variational integrators on Lagrangian systems

As we said previously, a direct discrete embedding is only based on the form of the
differential operator which is dependent of the coordinates system. Then, arises the natural
question of conservation of intrinsic properties of the differential equation at the discrete
level. This paper is devoted to the conservation of the Lagrangian structure. In this section,
we introduce variational integrators in the framework of the discrete embedding $FDE\sigma$.

3.1. Discrete calculus of variations and discrete embeddings. — In this subsection, we recall the strategy of variational integrators which are discretizations of Lagrangian
systems preserving their Lagrangian structures. It consists in building the discrete analog-
ous of the variational principle on a discretized Lagrangian functional. For more details,
we refer to [17] and [21]. In our case, the discrete Lagrangian functional is obtained by
giving a discrete embedding as defined in section 1.

3.1.1. Discrete Lagrangian functionals. — Giving $FDE\sigma$ induces the discretization of a
Lagrangian functional as long as a quadrature formula is fixed in order to approximate
integrals (as in (2.1)). We choose the usual $\sigma$-quadrature formula of Gauss:
for a continuous function $f$ on $[a, b]$, we discretize $\int_a^b f(t)dt$ by
\[
\sum_{k=0}^{N-1} (t_{k+1} - t_k) f(t_k) = h \sum_{k=0}^{N-1} f(t_k) \text{ if } \sigma = +
\]
and:
\[
\sum_{k=1}^{N} (t_k - t_{k-1}) f(t_k) = h \sum_{k=1}^{N} f(t_k) \text{ if } \sigma = -.
\]
This process defines the Gauss finite differences embedding which we denote by
Gauss-$FDE\sigma$. We can now define the following discrete Lagrangian functional:

Definition 7. — Let $\mathcal{L}$ be a Lagrangian functional associated to the Lagrangian $L$. The
discrete Lagrangian functional associated to $\mathcal{L}$ with respect to the discrete embedding
Gauss-$FDE\sigma$ is given by:
\[
\mathcal{L}_\sigma^\rho : (\mathbb{R}^d)^{N+1} \rightarrow \mathbb{R}
Q = (Q_i)_{i=0,...,N} \mapsto h \sum_{k \in I} L(Q_k, (-\sigma \Delta_{\sigma} Q)_k, t_k)
\]
where $I_+ = \{0,...,N-1\}$ and $I_- = \{1,...,N\}$.

Example 2. — Let us consider the Lagrangian functional associated to the mechanical
Lagrangian given by:
\[
\mathcal{L} : \mathcal{C}^2([a, b], \mathbb{R}^d) \rightarrow \mathbb{R}
q \mapsto \int_a^b \frac{1}{2} \dot{q}(t)^2 - U(q(t)) \, dt.
\]
Then, the discrete Lagrangian functional associated to $\mathcal{L}$ with respect to the discrete embedding Gauss-FDE is given by:

\[(3.1)\quad \mathcal{L}_h^− : (\mathbb{R}^d)^{N+1} \rightarrow \mathbb{R} \quad Q = (Q_i)_{i=0,...,N} \mapsto h \sum_{k=1}^{N} \frac{1}{2} \left(\frac{Q_k - Q_{k-1}}{h}\right)^2 - U(Q_k).\]

### 3.1.2. Discrete calculus of variations

Let $\mathcal{L}$ be a Lagrangian functional and $\mathcal{L}_h^\sigma$ the discrete Lagrangian functional associated with respect to Gauss-FDE$\sigma$. A discrete extremal (or discrete critical point) of $\mathcal{L}_h^\sigma$ is an element $Q$ in $(\mathbb{R}^d)^{N+1}$ such that $D\mathcal{L}_h^\sigma(Q)(W) = 0$ for any discrete variations $W$ (i.e. $W \in (\mathbb{R}^d)^{N+1}$, $W_0 = W_N = 0$).

Discrete extremals of $\mathcal{L}_h^\sigma$ can be characterized as solution of a system of equations:

**Theorem 2 (Discrete variational principle).** — Let $\mathcal{L}_h^\sigma$ be the discrete Lagrangian functional associated to the Lagrangian $\mathcal{L}$ with respect to Gauss-FDE$\sigma$. Then, $Q$ in $(\mathbb{R}^d)^{N+1}$ is a discrete extremal of $\mathcal{L}_h^\sigma$ if and only if $Q$ is solution of the following system of equations (called discrete Euler-Lagrange equation) given by:

\[(EL_h) \quad \frac{\partial L}{\partial x}(Q, -\sigma \Delta_\sigma Q, \tau) - \sigma \Delta_{-\sigma} \left(\frac{\partial L}{\partial v}(Q, -\sigma \Delta_\sigma Q, \tau)\right) = 0, \quad Q \in (\mathbb{R}^d)^{N+1}.\]

Thus, the variational integrator with respect to Gauss-FDE$\sigma$ on $[EL]$ is the numerical scheme $[EL_h]$; it corresponds to the discrete variational principle on the discrete Lagrangian functional defined with respect to Gauss-FDE$\sigma$.

**Example 3.** — As in example 2, let us consider the Lagrangian $(\star)$. The Gauss-FDE—leads to the discrete Lagrangian functional $\mathcal{L}_h^\sigma$ given by $(3.1)$. The discrete variational calculus on $\mathcal{L}_h^\sigma$ gives the associated discrete Euler-Lagrange equation:

\[\forall k \in 1, ..., N - 1, \quad \frac{Q_{k+1} - 2Q_k + Q_{k-1}}{h^2} = -\nabla U(Q_k), \quad Q \in (\mathbb{R}^d)^{N+1}.\]

The proof of theorem 2([L7]) is based on the following result:

**Lemma 1 (Discrete integration by parts).** — For any $F$ and $G$ in $(\mathbb{R}^d)^{N+1}$, we have:

\[\sum_{k=1}^{N} (\Delta_- F)_k G_k = \sum_{k=0}^{N-1} F_k (\Delta_+ G)_k + \frac{1}{h} (f_N g_N - f_0 g_0).\]

Discrete integration by parts emphasizes the asymmetric property of discrete operators $\Delta_+$ and $\Delta_-$ which does not exist in the continuous space with the operator $\frac{d}{dt}$. This characteristic leads to an asymmetry in $[EL_h]$; indeed, we have a composition between the two discrete operators $\Delta_+$ and $\Delta_-$. We notice that this asymmetry does not appear in the continuous space in $[EL]$. 
3.2. No coherence between direct discrete embedding and variational integrator. — We resume in figure 1 the previous processes in the setting of Gauss-FDEσ. We are interested in the coherence or not of this discrete embedding: do the direct discrete embedding and the variational integrator lead to the same numerical scheme for the Euler-Lagrange equation?

![Diagram](image)

Figure 1. No coherence between direct discrete embedding and variational integrator of the Euler-Lagrange equation in the setting of Gauss-FDEσ.

The previous study leads to a default of coherence of Gauss-FDEσ. Indeed, algorithms obtained by direct discrete embedding (2.2) and obtained by discrete variational principle (ELh) do not coincide. A temporal asymmetry appears in (ELh) which comes (mathematically) from lemma 1. The direct discrete embedding respects the law of semi-group of the differential operator \( \frac{d}{dt} \):

\[
\frac{d^2}{dt^2} = \frac{d}{dt} \circ \frac{d}{dt} \overset{\text{discretization}}{\rightarrow} (-\sigma \Delta_\sigma) \circ (-\sigma \Delta_\sigma) = \Delta_\sigma^2.
\]

As it is well-known from the numerical analysis point of view, [9], the composition of the discrete operator \(-\sigma \Delta_\sigma\) provides unstable numerical schemes. We loose the order of approximation of differential operator by composition: indeed, \(\Delta_\sigma^2\) approaches \(\frac{d^2}{dt^2}\) with an order 1 and not an order 2.

On the contrary, a variational integrator is not based on the algebraic construction of the differential equation via the differential operator but mainly on a dynamical approach via the extremals of a functional. As a consequence, the discrete Euler-Lagrange equation (ELh) does not necessary respect the algebraic property of composition. Nevertheless, the variational integrator uses the composition of discrete operators \(-\Delta_+\) and \(-\Delta_-\) and this composition provides an approximation of \(\frac{d^2}{dt^2}\) with an order 2.

The problem is to understand why this asymmetry does not appear with direct discrete embedding? It seems that we miss dynamical informations in the formulation of
Lagrangian systems at the continuous level which are pointed up in the discrete space with the asymmetric discrete operators \((-\sigma \Delta_\sigma)_{\sigma=\pm}\).

This default of coherence can be corrected using a different writing of the initial Euler-Lagrange equation. Indeed, we introduce in section 4 differential operators which conserve the temporal asymmetry in the continuous space: namely the asymmetric derivatives.

4. Discrete embedding of asymmetric Lagrangian systems

The usual way to derive differential equations in Physics is to build a continuous model using discrete data. However, this process gives only an information in one direction of time. As a consequence, a discrete evaluation of the velocity corresponds in general at the continuous level to the evaluation of the right or left derivative. In general, we replace the right (or left) derivative by the classical derivative \(\frac{d}{dt}\). However, this procedure assumes that the underlying solution is differentiable. This assumption is not only related to the regularity of the solutions but also to the reversibility of the systems (the right and left derivatives are equal). In this section, we introduce asymmetric Lagrangian systems which are obtained with functionals depending only on left or only on right derivatives. We prove in this case that \(Gauss-FDE_\sigma\) is coherent.

4.1. Asymmetric notations and asymmetric integration by parts. — Like operators \(-\Delta_+\) and \(\Delta_-\), we define differential operators which use only either future informations or past informations. They are just the minus right and the left classical derivatives:

**Definition 8** — For \(f : [a,b] \rightarrow \mathbb{R}^d\) smooth enough function, we denote:

\[
\forall t \in [a,b], \quad d_+ f(t) = \lim_{h \to 0^+} \frac{f(t) - f(t + h)}{h}
\]

and

\[
\forall t \in [a,b], \quad d_- f(t) = \lim_{h \to 0^+} \frac{f(t) - f(t - h)}{h}.
\]

Of course, for a differentiable function \(f\), we have \(d_- f = -d_+ f = \dot{f}\). However, as we are going to see in the next subsection, it is interesting to use these notations in order to keep dynamical informations.

**Lemma 2** (Asymmetric integration by parts). — For \(f, g : [a,b] \rightarrow \mathbb{R}^d\) smooth enough functions, we have:

\[
\int_a^b d_- f(t)g(t)dt = \int_a^b f(t)d_+ g(t)dt + f(b)g(b) - f(a)g(a).
\]

Let us notice that the asymmetric integration by parts is the continuous analogous of the discrete integration by parts (see lemma 1).
4.2. Asymmetric Lagrangian systems. — In this section, we introduce asymmetric Lagrangian systems which take into account the temporal asymmetry by using the differential operator $-\sigma d_\sigma$.

**Definition 9.** An asymmetric Lagrangian functional is an application:

$$L^\sigma : C^2([a, b], \mathbb{R}^d) \rightarrow \mathbb{R}$$

$$q \mapsto \int_a^b L(q(t), -\sigma d_\sigma q(t), t) \, dt$$

where $L$ is a Lagrangian.

Then, we obtain the following characterization of the extremals of an asymmetric Lagrangian functional as solution of an asymmetric differential equation:

**Theorem 3 (Variational principle).** Let $L^\sigma$ be an asymmetric Lagrangian functional associated to the Lagrangian $L$ and let $q \in C^2([a, b], \mathbb{R}^d)$. Then, $q$ is an extremal of $L^\sigma$ if and only if $q$ is solution of the asymmetric Euler-Lagrange equation:

$$(EL_\sigma) \ \forall t \in [a, b], \ \frac{\partial L}{\partial q}(q(t), -\sigma d_\sigma q(t), t) - \sigma d_{-\sigma} \left( \frac{\partial L}{\partial v}(q, -\sigma d_\sigma q, .) \right)(t) = 0.$$ 

Indeed, by using the asymmetric integration by parts in the proof of theorem 3, the asymmetry appears in $(EL_\sigma)$. Its origin is the continuous analogous of the asymmetry in $(EL_h)$. Now, we are interested in discrete embeddings of the asymmetric Euler-Lagrange equation.

4.3. Direct discrete embeddings and variational integrators of asymmetric Lagrangian systems. — In order to discretize $(EL_\sigma)$, we have to discretize two differential operators at the same time. In the discrete space, we replace the differential operator $d_+$ (respectively $d_-$) by $\Delta_+$ (respectively by $\Delta_-$). Then, we obtain an asymmetric version of the Gauss finite differences embedding mixing $\Delta_+$ and $\Delta_-:

**Definition 10.** We call the asymmetric Gauss-FDE$\sigma$ embedding the definition of the following elements: the application

$$\text{disc} : C^0([a, b], \mathbb{R}^d) \rightarrow (\mathbb{R}^d)^{N+1}$$

$$q \mapsto (q(t_i))_{i=0}^{N} = (Q_i)$$

the $\sigma$-quadrature formula of Gauss and the discrete operators

$$\Delta_+ : (\mathbb{R}^d)^{N+1} \rightarrow (\mathbb{R}^d)^N$$

$$Q = (Q_i)_{i=0}^{N} \mapsto \left( \frac{Q_i - Q_{i+1}}{h} \right)_{i=0}^{N-1}$$

and

$$\Delta_- : (\mathbb{R}^d)^{N+1} \rightarrow (\mathbb{R}^d)^N$$

$$Q = (Q_i)_{i=0}^{N} \mapsto \left( \frac{Q_i - Q_{i-1}}{h} \right)_{i=1}^{N}$$

These discrete operators are respectively the discrete versions of the operators $d_+$ and $d_-$ in the asymmetric Gauss-FDE$\sigma$. 

Definition 11. — Let $L$ be a Lagrangian and $[EL_\sigma]$ the asymmetric Euler-Lagrange equation associated. The direct discrete embedding of $[EL_\sigma]$ with respect to the asymmetric Gauss-FDE$\sigma$ is given by:

$$\frac{\partial L}{\partial x}(Q, -\sigma \Delta_\sigma Q, \tau) - \sigma \Delta_{-\sigma} \left( \frac{\partial L}{\partial v}(Q, -\sigma \Delta_\sigma Q, \tau) \right) = 0, \quad Q \in (\mathbb{R}^d)^{N+1}.$$ 

Let us notice that the direct discrete embedding of the asymmetric Euler-Lagrange equation gives the discrete Euler-Lagrange equation $[EL_h]$ (see definition 2). Obviously, as the asymmetric Gauss-FDE$\sigma$ gives the same discrete Lagrangian functional as the symmetric case, we deduce the coherence of this discrete embedding.

We notice that the asymmetric Gauss-FDE$\sigma$ unifies the algebraic approach and the dynamical approach in order to discretize Lagrangian systems. Indeed, the discrete and continuous versions of the asymmetric differential operators satisfy the same algebraic properties (temporal asymmetry, asymmetric integration by parts,...).

5. Introduction to fractional calculus

5.1. Notions of Grünwald-Letnikov and Riemann-Liouville. — Fractional calculus is the generalization of the derivative notion to real orders. There are many ways generalize this notion. We can generalize the derivative of a monomial and then generalize the derivative of functions which can be written in power series. We can do the same thing by generalizing derivative of an exponential or again derivative of cosinus and sinus. We can also use a generalization of the derivative by using a convolution. For more details, we refer to [19].

In this paper, we are going to use the classical notions of Grünwald-Letnikov and Riemann-Liouville. The following definitions and results are extracted from [22].

5.1.1. Fractional derivatives of Grünwald-Letnikov. — The notion of Grünwald-Letnikov comes from this simple result proved by induction:

let $f$ be a smooth enough function defined on $[a,b]$ and let $n \in \mathbb{N}$, then:

$$\forall t \in [a,b], \quad f^{(n)}(t) = \lim_{h \to 0^+} \frac{1}{h^n} \sum_{r=0}^{n} (-1)^r C_r^\alpha f(t - rh),$$

where $C_r^\alpha = \frac{n(n-1)...(n-r+1)}{r!}$. From this formula, Grünwald-Letnikov obtains this following generalization:

Definition 12. — Let $\alpha > 0$ and let $f$ be an element of $C^{n+1}([a,b], \mathbb{R}^d)$ where $n = [\alpha]$. Grünwald-Letnikov fractional left derivative of order $\alpha$ with inferior limit $a$ of $f$ is:

$$\forall t \in [a,b], \quad D_\alpha^a f(t) = \lim_{h \to 0^+} \frac{1}{h^\alpha} \sum_{r=0}^{n} (-1)^r C_r^\alpha f(t - rh).$$
Grünwald-Letnikov fractional right derivative of order $\alpha$ with superior limit $b$ of $f$ is:

$$\forall t \in [a, b[, \quad D_+^\alpha f(t) = \lim_{h \to 0} \frac{1}{h^\alpha} \sum_{r=0}^{n} (-1)^r C_r^\alpha f(t + rh).$$

5.1.2. Fractional derivatives of Riemann-Liouville. — The notion of Riemann-Liouville comes from this other simple result proved by induction:

let $f$ be a continuous function on $[a, b]$, let $t$ in $[a, b]$ and let $n \in \mathbb{N}$, then:

$$\int_a^t \int_a^{t_1} \ldots \int_a^{t_{n-1}} f(t_n)dt_n \ldots dt_1 = \frac{1}{(n-1)!} \int_a^t (t-y)^{n-1} f(y)dy.$$

From this formula, Riemann-Liouville obtains a generalization of the integral notion:

**Definition 13.** — Let $\alpha > 0$ and let $f$ be a continuous function.

Riemann-Liouville fractional left integral of order $\alpha$ with inferior limit $a$ is:

$$\forall t \in [a, b], \quad RL D^{-\alpha}_- f(t) := \frac{1}{\Gamma(\alpha)} \int_a^t (t-y)^{\alpha-1} f(y)dy.$$

Riemann-Liouville fractional right integral of order $\alpha$ with superior limit $b$ is:

$$\forall t \in [a, b], \quad RL D^{-\alpha}_+ f(t) := \frac{1}{\Gamma(\alpha)} \int_t^b (y-t)^{\alpha-1} f(y)dy.$$

where $\Gamma$ is the Gamma function which is an extension of the factorial function.

Finally, Riemann and Liouville obtain a generalization of the derivative notion by deriving fractional integrals:

**Definition 14.** — Let $\alpha > 0$ and let $f$ be an element of $C^{n+1}([a, b], \mathbb{R}^d)$ where $n = [\alpha]$.

Riemann-Liouville fractional left derivative of order $\alpha$ with inferior limit $a$ is:

$$\forall t \in [a, b], \quad RL D^\alpha_- f(t) := \frac{d^{n+1}}{dt^{n+1}} \left( RL D^{\alpha-(n+1)}_- f \right)(t).$$

Riemann-Liouville fractional right derivative of order $\alpha$ with superior limit $b$ is:

$$\forall t \in [a, b], \quad RL D^\alpha_+ f(t) := \frac{d^{n+1}}{dt^{n+1}} \left( RL D^{\alpha-(n+1)}_+ f \right)(t).$$

5.2. Links between these different notions. — Although the two approaches are different, they are linked by the following result, [22]:

**Theorem 4.** — Let $\alpha > 0$, $a < b$ two reals and $n = [\alpha]$. Let $f$ be a function in $C^{n+1}([a, b], \mathbb{R}^d)$ then the notion of fractional derivative of Riemann-Liouville and the one of Grünwald-Letnikov coincide. So we denote:

$$RL D^\alpha_+ f(t) = D^\alpha f(t)$$

and

$$RL D^\alpha_- f(t) = D^\alpha f(t).$$
Now, the following result proves that the Riemann-Liouville’s and the Grünwald-Letnikov’s fractional derivative notion is actually an extension of the classical derivative notion:

**Proposition 1.** — Let \( n \in \mathbb{N}^* \) and \( f \) be an element of \( \mathcal{C}^{n+1}([a,b], \mathbb{R}^d) \). Then, the following equalities hold:

\[
D_n^- f = f^{(n)} \quad \text{and} \quad D_n^+ f = (-1)^n f^{(n)}
\]

There exist fractional left derivatives and fractional right derivatives: this notion takes into account the temporal asymmetry. Moreover, there exists a formula of fractional integration by parts:

**Lemma 3 (Fractional integration by parts).** — Let \( 0 < \alpha < 1 \) and let \( f \) and \( g \) be two functions in \( \mathcal{C}^1([a,b], \mathbb{R}^d) \). We suppose that \( f(a) = f(b) = 0 \) or \( g(a) = g(b) = 0 \). Then, we have:

\[
\int_a^b D_\alpha^- f(y)g(y)dy = \int_a^b f(y)D_\alpha^+ g(y)dy.
\]

Let us notice that the fractional integration by parts is the fractional analogous of lemma 2, it transforms right fractional derivative into left fractional derivative. We will see that we have same behaviors in the discrete space with the discretized fractional operators (see lemma 4).

## 6. Discrete embeddings of fractional Lagrangian systems

In recent years, an important activity has been devoted to fractional Lagrangian systems for the purpose of optimal control, mechanics, engineering and Physics ([2], [4], [16]). There also exist many studies concerning the discretization of fractional differential equations ([2], [6], [3], [7], [8]).

In this section, following our previous approach on classical Lagrangian systems, we define fractional discrete embeddings and fractional variational integrators. We prove that a fractional discrete embedding is coherent.

### 6.1. Fractional Lagrangian systems.

**Definition 15.** — A fractional Lagrangian functional of order \( 0 < \alpha < 1 \) is an application defined by:

\[
\mathcal{L}_\sigma : \mathcal{C}^2([a,b], \mathbb{R}^d) \rightarrow \mathbb{R} \\
q \mapsto \int_a^b L(q(t), -\sigma D_\sigma^\alpha q(t), t)dt
\]

where \( L \) is a Lagrangian.

We can give a characterization of extremals of a fractional Lagrangian functional as solutions of a fractional differential equation:
Theorem 5 (Variational principle). — Let $\mathcal{L}^\sigma$ be a fractional Lagrangian functional of order $0 < \alpha < 1$ associated to the Lagrangian $L$ and let $q$ be an element of $C^2([a, b], \mathbb{R}^d)$. Then, $q$ is an extremal of $\mathcal{L}^\sigma$ if and only if $q$ is solution of the fractional Euler-Lagrange equation:

\[
(EL_f) \quad \forall t \in ]a, b[, \quad \frac{\partial}{\partial t}L(q(t), -\sigma D^\sigma_q(q(t), t) - \sigma D^\sigma_{-\sigma}(q, -\sigma D^\sigma_q, .)) (t) = 0.
\]

As in the asymmetric case, by using the fractional integration by parts, we obtain a fractional differential equation which presents a temporal asymmetry. Indeed, in $(EL_f)$, we have a composition of the $D^\alpha_+$ operator and the $D^\alpha_{-\sigma}$ operator.

6.2. Direct Gauss Grünwald-Letnikov embeddings of fractional Lagrangian systems. — We are interested in discrete embeddings of fractional Lagrangian systems. By referring to the notion of Grünwald-Letnikov ([15]), we give the following definition:

Definition 16. — The Gauss Grünwald-Letnikov embedding denoted by Gauss-GLE$\sigma$ the definition of the following elements: the application

\[
disc : \quad \mathcal{C}^0([a, b], \mathbb{R}^d) \longrightarrow (\mathbb{R}^d)^{N+1}, \quad q \mapsto (q(t_i))_{i=0,\ldots,N}
\]

the $\sigma$-quadrature formula of Gauss and the discrete operators

\[
\Delta^\alpha_- : \quad (\mathbb{R}^d)^{N+1} \longrightarrow (\mathbb{R}^d)^N
\]

\[
Q = (Q_k)_{k=0,\ldots,N} \mapsto \left(\frac{1}{h^\alpha} \sum_{r=0}^{k} (-1)^r C^r_\alpha Q_{k-r}\right)_{k=1,\ldots,N}
\]

and

\[
\Delta^\alpha_+ : \quad (\mathbb{R}^d)^{N+1} \longrightarrow (\mathbb{R}^d)^N
\]

\[
Q = (Q_k)_{k=0,\ldots,N} \mapsto \left(\frac{1}{h^\alpha} \sum_{r=0}^{N-k} (-1)^r C^r_\alpha Q_{k+r}\right)_{k=0,\ldots,N-1}
\]

These discrete operators are respectively discretized operators of the operators $D^\alpha_-$ and $D^\alpha_{-\sigma}$.

With such discrete operators, we have a formula of discrete fractional integration by parts which is exactly the discrete analogous of the fractional integration by parts at the continuous level (see lemma 3):

Lemma 4 (Discrete fractional integration by parts). — Let $F$ and $G$ be elements of $(\mathbb{R}^d)^{N+1}$ such that $F_0 = F_N = 0$ or $G_0 = G_N = 0$. Then, we have:

\[
\sum_{k=1}^{N} (\Delta^\alpha_- F)_k G_k = \sum_{k=0}^{N-1} F_k (\Delta^\alpha_+ G)_k.
\]

Proof. — The proof of this lemma is only based on the inversions of the two sums and on substitution of variables in the sums. We prove the lemma only in the case $F_0 = F_N = 0$. 

The case \( G_0 = G_N = 0 \) is similar.

As \( F_N = 0 \), we can sum \( k \) from 0 to \( N \) and we obtain by definition of \( (\Delta^*_+ \alpha G) \):

\[
\sum_{k=0}^{N-1} F_k(\Delta^*_+ \alpha G)_k = \frac{1}{\h} \sum_{k=0}^{N} \sum_{r=0}^{N-k} (-1)^r C^r \alpha F_k G_{k+r}
\]

\[
= \frac{1}{\h} \sum_{r=0}^{N} \sum_{k=0}^{N-r} (-1)^r C^r \alpha F_k G_{k+r}
\]

\[
= \frac{1}{\h} \sum_{r=0}^{N} \sum_{k=r}^{N} (-1)^r C^r \alpha F_{k-r} G_k
\]

\[
= \frac{1}{\h} \sum_{k=0}^{N} \sum_{r=0}^{k} (-1)^r C^r \alpha F_{k-r} G_k
\]

Then, as \( F_0 = 0 \), we can sum \( k \) only from 1 to \( N \) and we obtain:

\[
\sum_{k=1}^{N} F_k(\Delta^*_+ \alpha G)_k = \sum_{k=1}^{N} G_k \frac{1}{h^n} \sum_{r=0}^{k} (-1)^r C^r \alpha F_{k-r}
\]

\[
= \sum_{k=1}^{N} (\Delta^*_+ F)_k G_k.
\]

As in the asymmetric case, we notice that fractional operators and their discretized take into account the temporal asymmetry. The integration by parts on these operators leads to the same behavior: the fractional right derivative is transformed into the fractional left derivative. Then, we can expect the coherence of Gauss-GLE\( \sigma \). Now, let us give the definition of the direct discrete embedding of \( (EL_f) \) with respect to Gauss-GLE\( \sigma \):

**Definition 17.** — Let \( 0 < \alpha < 1 \) and let \( L \) be a Lagrangian and \( (EL_f) \) the fractional Euler-Lagrange equation associated to \( L \). The direct discrete embedding of \( (EL_f) \) with respect to Gauss-GLE\( \sigma \) is given by:

\[
(6.2) \quad \frac{\partial L}{\partial x} (Q, -\sigma \Delta^*_\alpha Q, \tau) - \sigma \Delta^*_\sigma \left( \frac{\partial L}{\partial v} (Q, -\sigma \Delta^*_\alpha Q, \tau) \right) = 0, \quad Q \in (\mathbb{R}^d)^{N+1}.
\]

### 6.3. Discrete calculus of variations on discrete fractional Lagrangian functionals.

Giving Gauss-GLE\( \sigma \) allows us to define the discretization of fractional Lagrangian functionals:

**Definition 18.** — Let \( 0 < \alpha < 1 \) and let \( \mathcal{L}^\sigma \) be the fractional Lagrangian functional associated to the Lagrangian \( L \). The discrete fractional Lagrangian functional associated to \( \mathcal{L}^\sigma \) with respect to the embedding Gauss-GLE\( \sigma \) is given by:

\[
\mathcal{L}^\sigma_h : \quad (\mathbb{R}^d)^{N+1} \rightarrow \mathbb{R}
\]

\[
Q = (Q_i)_{i=0,\ldots,N} \quad \rightarrow \quad h \sum_{k \in I_+} L(Q_k, (-\sigma \Delta^*_\alpha Q)_k, t_k),
\]

where \( I_+ = \{0, \ldots, N-1\} \) and \( I_- = \{1, \ldots, N\} \).

Discrete extremals of \( \mathcal{L}^\sigma_h \) can be characterized as solution of a system of equations:
Theorem 6 (Discrete variational principle). — Let $0 < \alpha < 1$ and let $\mathcal{L}_h^\alpha$ be a discrete fractional Lagrangian functional associated to the Lagrangian $L$ with respect to the discrete embedding Gauss-GLE$\sigma$. Then, $Q$ in $(\mathbb{R}^d)^{N+1}$ is a discrete extremal of $\mathcal{L}_h^\alpha$ if and only if $Q$ is solution of the following system of equations, called the **discrete fractional Euler-Lagrange equation**:

\[
(EL_{f,h}) \quad \frac{\partial L}{\partial x}(Q, -\sigma \Delta_\alpha^Q, \tau) - \sigma \Delta_\alpha^\sigma \left( \frac{\partial L}{\partial v}(Q, -\sigma \Delta_\alpha^Q, \tau) \right) = 0, \quad Q \in (\mathbb{R}^d)^{N+1}.
\]

**Proof.** We write the proof only in the case $\sigma = -$. The proof in the case $\sigma = +$ is similar.

Let $Q$ in $(\mathbb{R}^d)^{N+1}$ and $W$ a discrete variation of $(\mathbb{R}^d)^{N+1}$. Then:

\[
\mathcal{L}_h^-(Q + W) = h \sum_{k=1}^N L(Q_k + W_k, (\Delta_\alpha^\sigma)Q + (\Delta_\alpha^\sigma)W_k, t_k)
\]

\[
= \mathcal{L}_h^-(Q) + h \sum_{k=1}^N \frac{\partial L}{\partial x}(Q_k, (\Delta_\alpha^\sigma)Q_k, t_k)W_k + \frac{\partial L}{\partial v}(Q_k, (\Delta_\alpha^\sigma)Q_k, t_k)(\Delta_\alpha^\sigma)W_k + o(\|W\|)
\]

where $o$ is the Landau’s notation. Thus, by definition of the differential, we obtain:

\[
D\mathcal{L}_h^-(Q)(W) = h \sum_{k=1}^N \frac{\partial L}{\partial x}(Q_k, (\Delta_\alpha^\sigma)Q_k, t_k)W_k + \frac{\partial L}{\partial v}(Q_k, (\Delta_\alpha^\sigma)Q_k, t_k)(\Delta_\alpha^\sigma)W_k
\]

Since $W$ is a discrete variation of $(\mathbb{R}^d)^{N+1}$, $W_0 = W_N = 0$. By applying the discrete fractional integration by parts on the second term of the previous sum, we obtain:

\[
D\mathcal{L}_h^-(Q)(W) = 0 \iff h \sum_{k=1}^{N-1} \left( \frac{\partial L}{\partial x}(Q_k, (\Delta_\alpha^\sigma)Q_k, t_k) + (\Delta_\alpha^+(\frac{\partial L}{\partial v}(Q, (\Delta_\alpha^\sigma), \tau)))_k \right) W_k = 0.
\]

Thus, $Q$ is a discrete extremal of $\mathcal{L}_h^-$ if and only if $Q$ is solution of the discrete fractional Euler-Lagrange equation $(EL_{f,h})$ as defined in theorem 6.

As we expected before, we notice that we have coherence of the discrete embedding Gauss-GLE$\sigma$ of the fractional Euler-Lagrange equation. Indeed, formulas (6.2) and $(EL_{f,h})$ coincide.

### 7. Conclusion

In this paper, we have introduced the notion of discrete embeddings and constructed the corresponding variational integrators in the classical and fractional cases. The discrete embedding has to conserve the integration by parts on the discrete level in order to be coherent.

The Gauss finite differences embedding or Grünwald-Letnikov embedding are only here as illustration of our point of view. In order to construct more efficient numerical schemes,
one can choose appropriate discretization for the differential operators and also more elaborate quadrature formulas for integrals. In particular, we can have a look in [15] for special discretization of the fractional derivatives.

In [23], Riewe has introduced fractional Lagrangian functionals in order to model dissipative effects. However, his formalism does not provide an equivalence between solutions of a dissipative equation and critical points of fractional Lagrangian functional. Moreover, his construction is based on very stringent assumptions on functions. The asymmetric fractional calculus of variations (where the functional space is split in two) introduced in [13] solves this problem and provides a full equivalence between critical points of an asymmetric fractional Lagrangian functional and solutions of a dissipative system (as the linear friction case or the diffusion equation for example). A natural extension of our work is to extend the fractional discrete embedding to cover the asymmetric fractional case.

Several difficulties arise in the numerical study of the convection-diffusion equation, in particular the presence of non physical numerical oscillations for high values of the Reynolds number. An asymmetric fractional Lagrangian formulation of the convection-diffusion equation is obtained in [12]. Our idea is to construct an adapted fractional variational integrator in order to control the discrete solutions of the numerical scheme. This will be done in a forthcoming paper.
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