Discrete embeddings for Lagrangian and Hamiltonian systems

Jacky Cresson *[1], Isabelle Greff †[1] and Charles Pierre ‡[1]

[1] Laboratoire de Mathématiques et de leurs Applications, UMR CNRS 5142, Université de Pau et des Pays de l'Adour, France

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Abstract

The topic of this paper is to study the conservation of variational properties for a given problem when discretising it. Precisely we are interested in Lagrangian or Hamiltonian structures and thus with variational problems attached to a least action principle. Consider a partial differential equation (PDE) deriving from a variational principle. A natural question is to know whether this structure is preserved at the discrete level when discretising the PDE. To address this question a concept of *coherence* is introduced. Both the differential equation (the PDE translating the least action principle) and the variational structure can be embedded at the discrete level. This provides two discrete embeddings for the original problem. If these procedures finally provide the same discrete problem we will say that the discretisation is *coherent*. Our purpose is illustrated with the Poisson problem. Coherence for discrete embeddings of Lagrangian structures is studied for various classical discretisations. For Hamiltonian structures, we show the coherence between a discrete Hamiltonian and the discretisation of the mixed formulation of the Poisson problem.

*jacky.cresson@univ-pau.fr
†isabelle.greff@univ-pau.fr
‡charles.pierre@univ-pau.fr

Introduction

Many problems in physics, formulated in terms of Partial Differential Equations (PDE), are associated with essential structural properties. For instance we mention the maximum principle, conservation laws or variational principles in mechanics. It is quite natural to ask the numerical methods to preserve these structural properties at the discrete level: in order to enforce the numerical solutions to satisfy the underlying physics of the problem.

Two fundamental notions arising in classical mechanics are Lagrangian and Hamiltonian structures. Lagrangian systems are made of one functional, called the Lagrangian functional, and a variational principle called the least action principle. From the least action principle is derived a second order differential equation called the Euler-Lagrange equation, see e.g. [1]. The Lagrangian structure is much more fundamental than its associated Euler-Lagrange equation: it contains information that the Euler-Lagrange equation does not. An important example is the change of coordinates. The Lagrangian structure is independent from change of coordinates, whereas the associated Euler-Lagrange equation may completely change of nature (from linear to non linear for instance). Similarly, Hamiltonian systems also are associated to a variational structure. They are associated with fundamental properties such as energy conservation or existence of first integrals.

Consider a numerical method for the resolution of a problem that derives from a variational principle. When understanding how the original variational structure is embedded at the discrete level, one can answer how the associated properties will be preserved by the numerical solutions. There has been a wide range of works about the conservation of geometrical properties at the numerical level by Hairer *et al.* [17, 15, 16], by Faou [11] and on the conservation of variational structures by Marsden *et al.* [23, 18, 20, 19] in the case of ODEs.

In this paper we will analyse the question of the conservation of variational structure as follows. We consider the general framework of embeddings as presented in [5, 4, 6, 7]. We introduce the concept of *coherence*. Consider a problem associated to a Lagrangian structure. On one hand we have the Lagrangian functional $\mathcal{L}$ on a functional space. On the other hand we have the corresponding Euler-Lagrange equation. Discretisation can be performed in two different ways.

- Either by discretising the Euler-Lagrange equation. This will be called a *discrete differential embedding* because it is based on deriving discrete versions of the differential operators in this PDE.

- Or discretise the Lagrangian structure by defining a discrete Lagrangian functional $\mathcal{L}_h$ and the associated discrete least action principle. This second procedure is called *discrete variational embedding* (it is also called *variational integrator*).

In case the discrete differential embedding and the discrete variational embedding are equivalent, we will say that we have *coherence*. The same notion of coherence can be defined relatively to Hamiltonian structures.
In case of coherence, the numerical solutions will inherit the properties of the original physical problem (conservation of energy, independence with the coordinate system...).
Based on this notion of coherence, the present work is an attempt to interpret numerical methods as *variational integrators* for PDEs deriving from a Lagrangian/Hamiltonian structure. We will focus on a canonical example of such a problem: the Poisson equation. This problem is well documented at the continuous and at the discrete levels. It provides an appropriate test case to improve the understanding of discrete embeddings for Lagrangian/Hamiltonian structure.

The outline of the paper is as follows. In section 1 are presented Lagrangian systems. We introduce in section 2 the notions of discrete differential and discrete variational embeddings, and give various examples. The concept of coherence is then defined in section 2.4. In section 3, we study the coherence for finite difference and finite volume methods, as applied to the Poisson equation. Section 4 is concerned with Hamiltonian structures and mixed formulations. The discrete embedding of Hamiltonian structures is analysed for the mimetic finite difference method that is shown to be coherent.

Throughout this paper, $\Omega \subset \mathbb{R}^d$ is a bounded domain with regular boundary. The Sobolev space of order m is denoted by $\mathrm{H}^m(\Omega)$ and the two following spaces $\mathrm{H}^1_0(\Omega) = \left\{v \in \mathrm{H}^1(\Omega), v_{|\partial\Omega} = 0\right\}$, $\mathrm{H}_{\mathrm{div}}(\Omega) = \left\{\mathbf{p} \in [\mathrm{L}^2(\Omega)]^d,\ \operatorname{div}\mathbf{p} \in \mathrm{L}^2(\Omega)\right\}$ will be considered.

1 Lagrangian systems

We recall classical results about Lagrangian calculus of variations for PDEs, illustrated in section 1.2 with the Lagrangian formulation of the Poisson problem. For more details, we refer to [9, 12, 13].

1.1 Lagrangian calculus of variations

Definition 1. An admissible Lagrangian function L is a function,

$$\begin{array}{rcl} L : \Omega \times \mathbb{R} \times \mathbb{R}^d & \longrightarrow & \mathbb{R} \\ (x, y, z) & \mapsto & L(x, y, z), \end{array}$$

such that L is of class $\mathcal{C}^1$ with respect to y and z and integrable in x. The Lagrangian function L defines the *Lagrangian functional* $\mathcal{L}$:

$$\begin{array}{rcl} \mathcal{L} : \mathrm{H}^1(\Omega) & \to & \mathbb{R}, \\ u & \longmapsto & \displaystyle\int_\Omega L(x, u(x), \nabla u(x))\,\mathrm{d}x. \end{array}$$

We are interested to vanish the first variations of the Lagrangian functional $\mathcal{L}$ on a space of variations V. As in [12], we could give a general notion for extremals and variations. We take the following definitions of the notions of a differentiable functional and an extremal for $\mathcal{L}$.

Definition 2 (Differentiability)**.** We consider a space of variations $V \subset \mathrm{H}^1(\Omega)$. The functional $\mathcal{L}$ is *differentiable* at point $u \in \mathrm{H}^1(\Omega)$ if and only if the limit,

$$\lim_{\epsilon\to 0} \frac{\mathcal{L}(u+\epsilon v) - \mathcal{L}(u)}{\epsilon},$$

exists in any direction $v \in V$. We then define the differential $D\mathcal{L}(u)$ of $\mathcal{L}$ at point u as,

$$v \in V \mapsto D\mathcal{L}(u)(v) = \lim_{\epsilon\to 0} \frac{\mathcal{L}(u+\epsilon v) - \mathcal{L}(u)}{\epsilon}.$$

With the above definition of differentiability, one recovers the usual definition of the differential in case $V = \mathrm{H}^1(\Omega)$ and $D\mathcal{L}(u)$ is linear and continuous in u on $\mathrm{H}^1(\Omega)$. The definition given here suffices to introduce extremals:

Definition 3 (Extremals)**.** A function $u \in \mathrm{H}^1(\Omega)$ is an extremal for the functional $\mathcal{L}$ relatively to the space of variations $V \subset \mathrm{H}^1(\Omega)$ if $\mathcal{L}$ is differentiable at point u and:

$$D\mathcal{L}(u)(v) = 0 \quad \text{for any} \quad v \in V.$$

Proposition 1. If $x \mapsto \dfrac{\partial L}{\partial y}(x, u(x), \nabla u(x))$ and $x \mapsto \dfrac{\partial L}{\partial z}(x, u(x), \nabla u(x))$ respectively are in $\mathrm{L}^2(\Omega)$ and in $[\mathrm{L}^2(\Omega)]^d$, then the Lagrangian functional $\mathcal{L}$ is differentiable at point $u \in \mathrm{H}^1(\Omega)$.
In that case the differential is given for any $v \in \mathrm{H}^1(\Omega)$ by:

$$D\mathcal{L}(u)(v) = \int_\Omega \left[\frac{\partial L}{\partial y}\big(x, u(x), \nabla u(x)\big)\ v(x) + \frac{\partial L}{\partial z}\big(x, u(x), \nabla u(x)\big)\cdot \nabla v(x)\right] \mathrm{d}x. \tag{1}$$

Proof. Using a Taylor expansion of L at the point $(x, u+\epsilon v, \nabla(u+\epsilon v))$ in the variables y and z leads to:

$$L\big(x, u+\epsilon v, \nabla(u+\epsilon v)\big) = L(x, u, \nabla u) + \epsilon\, v\, \frac{\partial L}{\partial y}(x, u, \nabla u) + \nabla(\epsilon\, v)\cdot \frac{\partial L}{\partial z}(x, u, \nabla u) + o(\epsilon).$$

Integrating over the domain Ω gives:

$$\begin{aligned}\mathcal{L}(u+\epsilon v) = \mathcal{L}(u) &+ \epsilon \int_\Omega v(x)\frac{\partial L}{\partial y}(x, u(x), \nabla u(x))\mathrm{d}x \\ &+ \epsilon \int_\Omega \nabla v(x) \cdot \frac{\partial L}{\partial z}(x, u(x), \nabla u(x))\mathrm{d}x + o(\epsilon),\end{aligned}$$

leading to (1). $\square$

Extremals of the functional $\mathcal{L}$ can be characterised by an order 2 PDE, called the *Euler-Lagrange equation* given in the following theorem.

Theorem 1 (Least action principle)**.** Consider a Lagrangian functional $\mathcal{L}$ that satisfies the sufficient conditions of differentiability of proposition 1 at point $u \in \mathrm{H}^1(\Omega)$. Assume that u is an extremal for a given space of variations V and that $\frac{\partial L}{\partial z}(\cdot, u(\cdot), \nabla u(\cdot)) \in \mathrm{H}_{\mathrm{div}}(\Omega)$. Moreover the subspace $V_0 = \{v \in V, v = 0 \text{ on } \partial\Omega\}$ is supposed to be dense in $\mathrm{L}^2(\Omega)$. Then u satisfies the Euler-Lagrange equation:

$$\frac{\partial L}{\partial y}(x, u(x), \nabla u(x)) - \mathrm{div}\left(\frac{\partial L}{\partial z}(x, u(x), \nabla u(x))\right) = 0\,. \tag{2}$$

In the sequel we will denote P the differential operator associated to the Euler-Lagrange equation given by

$$P(u) := \frac{\partial L}{\partial y}(x, u(x), \nabla u(x)) - \mathrm{div}\left(\frac{\partial L}{\partial z}(x, u(x), \nabla u(x))\right). \tag{3}$$

Proof. Following (1) and using the Green formula gives: $\forall\ v \in V_0$,

$$\int_\Omega \left[\frac{\partial L}{\partial y}(x, u(x), \nabla u(x)) - \mathrm{div}\left(\frac{\partial L}{\partial z}(x, u(x), \nabla u(x))\right)\right] v(x)\mathrm{d}x = 0,$$

which implies (2) by density of V_0 in $\mathrm{L}^2(\Omega)$. $\square$

1.2 Lagrangian structure for the Poisson problem

We consider the Poisson problem on Ω for a homogeneous Dirichlet boundary condition: find $u \in \mathrm{H}^2(\Omega)$,

$$-\Delta u = f \quad \text{in} \quad \Omega, \quad \text{and} \quad u = 0 \quad \text{on} \quad \partial\Omega, \tag{4}$$

for a data $f \in \mathrm{L}^2(\Omega)$. Assuming that Ω is bounded with a smooth boundary, problem (4) has a unique solution $u \in \mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$.
Equation (4) is the differential formulation of the Poisson problem. Let us now present its variational formulation. We consider the Lagrangian function L:

$$L(x, y, z) = \frac{1}{2} z \cdot z - f(x)y.$$

The associated Lagrangian functional $\mathcal{L}$ is given by,

$$\mathcal{L}(u) = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 \; - \; fu \right) \mathrm{d}x\,. \tag{5}$$

The differential formulation (4) of the Poisson problem is equivalent to,

$$\text{find} \quad u \in \mathrm{H}^1_0(\Omega) \quad \text{so that} \quad \forall\, v \in \mathrm{H}^1_0(\Omega), \quad D\mathcal{L}(u)(v) = 0, \tag{6}$$

Equation (6) is the well-known variational formulation of the Poisson problem, with the space of variation $V = \mathrm{H}^1_0(\Omega)$ given by:

$$\int_\Omega \nabla u \, \nabla v \, \mathrm{d}x = \int_\Omega f \, v \mathrm{d}x\,.$$

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2 Discrete embeddings

The formalism of embeddings has been initiated in [5] and further developed in [4, 6, 7]. We propose here a general notion of discrete embeddings. This notion is defined in two particular cases: discrete embeddings of differential operators called discrete differential embedding in section 2.2 and discrete embeddings of Lagrangian functionals called discrete variational embedding in section 2.3. The notion of coherence between discrete differential and discrete variational embeddings is presented in section 2.4.

2.1 General definitions

Let X denote a functional space on Ω. We consider the mapping,

$$P : \; u \in X \mapsto P(u) \in Y,$$

where Y either is a functional space on Ω or $Y = \mathbb{R}$. At this point no particular property is required for P.

Definition 4. We consider X_h and Y_h two finite dimensional spaces and $\pi_1 : \; X \to X_h$, $\pi_2 : \; Y \to Y_h$ two surjective linear mappings. We introduce $P_h : \; X_h \to Y_h$ and consider the diagram:

$$\begin{array}{ccc} X & \xrightarrow{P} & Y \\ {\scriptstyle \pi_1}\downarrow & & \downarrow{\scriptstyle \pi_2} \\ X_h & \xrightarrow{P_h} & Y_h \end{array} \tag{7}$$

We say that P_h is a discrete embedding of P.

Remark 1. The setting presented in definition 4 is general. It introduces discrete (finite dimensional) counterparts for the functional spaces X and Y. These discrete spaces theirselves can be functional spaces (such as for finite element methods *e.g.*) or not (such as for finite difference methods). The diagram is not commutative in general.

Consider again the Poisson problem. On one hand we have its differential formulation (4). It is associated to the mapping $P:\ u \in X \mapsto \Delta u + f \in Y$, with $X = \mathrm{H}^2(\Omega)$ and $Y = \mathrm{L}^2(\Omega)$. The Poisson problem rewrites as:

$$\text{find} \quad u \in M \subset X \quad \text{so that} \quad P(u) = 0,$$

with $M = \mathrm{H}^1_0(\Omega) \cap X$. A discretisation for the differential formulation of the Poisson problem reads,

$$\text{find} \quad u_h \in M_h \subset X_h \quad \text{so that} \quad P_h(u_h) = 0, \tag{8}$$

where $P_h:\ X_h \to Y_h$ is a discrete embedding of P and where $M_h \subset X_h$ encodes the boundary condition. The definition of P_h requires a definition of Δ_h. This is a discrete embedding for the Laplace operator and will be referred as discrete differential embeddings. This is detailed in section 2.2.

On the other hand the variational formulation (6) of the Poisson problem, with $X = \mathrm{H}^1(\Omega)$, $\mathcal{L}:\ X \to \mathbb{R}$ and $V = \mathrm{H}^1_0(\Omega) = M$ rewrites as,

$$\text{find} \quad u \in M \subset X \quad \text{so that} \quad \forall\, v \in V, \quad D\mathcal{L}(u)(v) = 0.$$

A discretisation for the variational formulation of the Poisson problem reads:

$$\text{find} \quad u_h \in M_h \subset X_h \quad \text{so that} \quad \forall\, v_h \in V_h, \quad D\mathcal{L}_h(u_h)(v_h) = 0.$$

It involves $\mathcal{L}_h:\ X_h \to \mathbb{R}$, a discrete embedding of the Lagrangian functional $\mathcal{L}:\ X \to \mathbb{R}$, that will be referred as discrete variational embedding. This is developed in section 2.3.

2.2 Discrete differential embeddings

Definition 5. Consider the diagram (7) in definition 4 in the case where P is associated with some PDE $P(u) = 0$, *i.e.* P is a differential operator. In that particular case we call P_h a discrete differential embedding.

Note that a discrete differential embedding is not a differential operator itself. It is the discretisation of a differential operator.

Consider the discrete differential embedding for the Poisson problem (8). We set $P_h u_h = \Delta_h u_h + f_h$. The definition of P_h involves a definition of f_h and of Δ_h. Two ways can be followed to derive Δ_h. The first one is to directly discretise the Laplacian, as it is done using finite difference methods in section 3.1.

The second one is to use the divergence form of the Laplacian: $\Delta = \operatorname{div} \circ \nabla$ and to derive a discrete embedding for the Laplacian as $\Delta_h = \operatorname{div}_h \circ \nabla_h$, where div_h and ∇_h are two discrete differential embedding of div and ∇. This will be the case with finite volume methods in section 3.2.
This leads to two discrete differential embeddings for the Poisson problem: either,

$$-\Delta_h u_h = f_h,$$

or,

$$-\operatorname{div}_h(\nabla_h u_h) = f_h.$$

These two discrete problems do not coincide in general. Indeed, recovering the algebraic properties of the original differential operators (here $\Delta = \operatorname{div} \circ \nabla$) at the discrete level (here $\Delta_h = \operatorname{div}_h \circ \nabla_h$) is a full problem by itself.

We now give three illustrations of discrete differential embeddings: for the gradient operator and for the divergence one. Let us start precising the notion of a mesh for the domain $\Omega \subset \mathbb{R}^d$ $d = 2, 3$.

Definition 6 (Mesh)**.** A cell is a polygonal/polyhedral non empty open subset of $\mathbb{R}^d$. A mesh $\mathcal{T}$ of the domain Ω is a collection of cells partitioning Ω in the following sense:

$$\cup_{K\in\mathcal{T}}\overline{K} = \overline{\Omega}, \qquad \text{and} \qquad \Big(K_1, K_2 \in \mathcal{T} \;\Rightarrow\; \text{either} \quad K_1 \cap K_2 = \emptyset \quad \text{or} \quad K_1 = K_2\Big).$$

A face (or an edge) e of some $K \in \mathcal{T}$ such that $e \subset \partial\Omega$ is called a boundary face. The set of boundary faces is denoted $\mathcal{E}_0$. It satisfies: $\partial\Omega = \cup_{e\in\mathcal{E}_0} e$. For every $e \in \mathcal{E}_0$, there exists a unique $K \in \mathcal{T}$ satisfying $e \subset \overline{K} \cap \partial\Omega$: one writes $e = K|\partial\Omega$.
The internal faces set $\mathcal{E}_i$ associated with $\mathcal{T}$ is the set of all geometrical subsets $e = \overline{K_1} \cap \overline{K_2}$, $K_1, K_2 \in \mathcal{T}$ and $K_1 \neq K_2$, having non-zero $(d-1)-$dimensional measure. For every $e \in \mathcal{E}_i$, there exists a unique couple $K_1, K_2 \in \mathcal{T}$ satisfying $e = \overline{K_1} \cap \overline{K_2}$: one writes $e = K_1|K_2$.
The faces set associated with $\mathcal{T}$ is given as $\mathcal{E} = \mathcal{E}_0 \cup \mathcal{E}_i$. It provides a partitioning of $\cup_{K\in\mathcal{T}}\partial K$, in the same meaning as earlier: $\cup_{e\in\mathcal{E}} e = \cup_{K\in\mathcal{T}}\partial K$ and the overlapping of two distinct faces either is empty or of zero $(d-1)-$dimensional measure. Let $e \in \mathcal{E}$ such that $e \subset \partial K$ for $K \in \mathcal{T}$. We denote $\mathbf{n}_{K,e}$ the unit normal to e pointing outward of K. We also provide intrinsic orientation to faces: to all faces $e \in \mathcal{E}$ is associated $\mathbf{n}_e$ one of its (two) unit normal, if $e \subset \partial K$ we have $\mathbf{n}_e = \pm\mathbf{n}_{K,e}$.
The set of vertexes associated with $\mathcal{T}$ is denoted $\mathcal{N}$: it contains exactly all the vertexes of all the cells $K \in \mathcal{T}$.

One shall denote $|O|$ the measure of a geometrical object O according to its dimension. Taking $d = 3$, $|K|$ is the volume of the cell K, $|e|$ the area of an edge $e \in \mathcal{E}$ and $|xy|$ the length between two points x and y. The cardinal of a set E is $\#E$.

2.2.1 The finite volume divergence

We denote here $X = [\mathrm{H}^1(\Omega)]^d$, $Y = \mathrm{L}^2(\Omega)$ and $\mathrm{div}: X \to Y$ is the divergence operator. Let $\mathcal{T}$ be a mesh of Ω. We here define $X_h = \mathbb{R}^{\#\mathcal{E}}$, and $Y_h = P^0(\mathcal{T})$ the space of piecewise constant functions over the cells of the mesh, with the natural identification $Y_h = \mathbb{R}^{\#\mathcal{T}}$. Note that in general there is no natural identification of $\mathbb{R}^{\#\mathcal{E}}$ with some finite dimensional vector field space over Ω, we however mention the case of simplicial meshes where such an identification is provided by the Raviart-Thomas finite element space of order 0, $RT_0(\Omega)$, see [21].
To $\mathbf{p} \in X$ we associate $\pi_1 \mathbf{p} = (p_e)_{e\in\mathcal{E}}$ with $p_e = \int_e \mathbf{p}\cdot\mathbf{n}_e \mathrm{d}l/|e|$ the mean flux of $\mathbf{p}$ across the face e according to its orientation provided by $\mathbf{n}_e$ (in the trace sense). To $f \in \mathrm{L}^2(\Omega)$, we associate $\pi_2 f = (f_K)_{K\in\mathcal{T}}$ with $f_K = \int_K f\,\mathrm{d}x/|K|$ the mean value of f on the cell K. The discrete divergence is defined as,

$$\mathrm{div}_h: \ \mathbf{p}_h = (p_e)_{e\in\mathcal{E}} \in \mathbb{R}^{\#\mathcal{E}} \mapsto (\mathrm{div}_K\, \mathbf{p}_h)_{K\in\mathcal{T}} \in \mathbb{R}^{\#\mathcal{T}},$$

with,

$$\mathrm{div}_K\, \mathbf{p}_h = \frac{1}{|K|} \sum_{e\in\mathcal{E}, e\subset\partial K} p_e |e|\ \mathbf{n}_e \cdot \mathbf{n}_{K,e}. \tag{9}$$

This definition simply is the flux balance around the cell K, the last term $\mathbf{n}_e\cdot\mathbf{n}_{K,e}$ giving the correct orientation for the fluxes, *i.e.* outside the cell K.

With these definitions we have a discrete differential embedding for the divergence,

$$\begin{array}{ccc} [\mathrm{H}^1(\Omega)]^d & \xrightarrow{\mathrm{div}} & \mathrm{L}^2(\Omega) \\ {\scriptstyle \pi_1}\big\downarrow & & \big\downarrow{\scriptstyle \pi_2} \\ \mathbb{R}^{\#\mathcal{E}} & \xrightarrow{\mathrm{div}_h} & R^{\#\mathcal{T}} \end{array} \tag{10}$$

and this diagram moreover is commutative thanks to the divergence formula: $\pi_2 \circ \mathrm{div} = \mathrm{div}_h \circ \pi_1$.

2.2.2 The $P^1(\mathcal{T})$ finite element gradient

We introduce $X = C^1(\Omega)$ and $Y = [C^0(\Omega))]^d$ the spaces of continuously differentiable functions and of continuous vector fields over Ω respectively. We now consider the gradient operator $\nabla: \ C^1(\Omega) \to [C^0(\Omega)]^d$.
Let $X_h = P^1(\mathcal{T})$ be the space of continuous functions over Ω that moreover are piecewise affine on each cell $K \in \mathcal{T}$. Let us assume that the mesh is simplicial, the space X_h is identified to $\mathbb{R}^{\#\mathcal{N}}$. We have the projection $\pi_1: \ u \in C^1(\Omega) \mapsto \pi_1 u = (u_S)_{S\in\mathcal{N}} \in P^1(\mathcal{T})$ with $u_S = u(S)$. Let $Y_h = [P^0(\mathcal{T})]^d$ be the space of piecewise constant vector fields over each cell $K \in \mathcal{T}$. We have a simple projection $\pi_2: \ [C^0(\Omega)]^d \to [P^0(\mathcal{T})]^d$ by averaging a vector field over each cell of the mesh (similarly to π_2 in section 2.2.1).

We have the following discrete differential embedding for the gradient:

$$\begin{array}{ccc} C^1(\Omega) & \xrightarrow{\nabla} & [C^0(\Omega))]^d \\ {\scriptstyle \pi_1}\big\downarrow & & \big\downarrow{\scriptstyle \pi_2} \\ P^1(\mathcal{T}) & \xrightarrow{\nabla_h} & [P^0(\mathcal{T})]^d \end{array} \tag{11}$$

where the discrete gradient $\nabla_h = \nabla_{|P^1(\mathcal{T})}$ indeed is the restriction of the continuous one to $P^1(\mathcal{T})$. In that case the diagram is not commutative.

2.2.3 Non-conforming finite element gradient

We propose a second definition of discrete differential embedding of the gradient, that is referred to as *non-conforming finite element gradient* since it matches with the Crouzeix-Raviart finite element of order 1 discretisation, see [8], in the case of a simplicial mesh.
Let $X = \mathrm{H}^1(\Omega)$, $Y = [\mathrm{L}^2(\Omega)]^d$ and consider $\nabla :\ \mathrm{H}^1(\Omega) \to [\mathrm{L}^2(\Omega)]^d$. We set $X_h = \mathbb{R}^{\#\mathcal{E}}$ and $Y_h = [P^0(\mathcal{T})]^d$ the space of piecewise constant vector fields over the cells of the mesh, with the natural identification $Y_h = \left[\mathbb{R}^d\right]^{\#\mathcal{T}}$. To $u \in \mathrm{H}^1(\Omega)$ we associate $\pi_1 u = (u_e)_{e\in\mathcal{E}}$ with $u_e = \int_e u \mathrm{d}l/|e|$ the mean value of u on the face e (in the trace sense). We have the same simple projection $\pi_2 :\ [\mathrm{L}^2(\Omega)]^d \to \left[\mathbb{R}^d\right]^{\#\mathcal{T}}$ as in section 2.2.2 by averaging a vector field over each cell of the mesh. The discrete gradient is defined as,

$$\nabla_h :\ u_h = (u_e)_{e\in\mathcal{E}} \in X_h \mapsto (\nabla_K u_h)_{K\in\mathcal{T}} \in \left[\mathbb{R}^d\right]^{\#\mathcal{T}},$$

with,

$$\nabla_K u_h = \frac{1}{|K|} \sum_{e\in\mathcal{E}, e\subset\partial K} u_e |e|\ \mathbf{n}_{K,e}.$$

With these definitions we have the following discrete differential embedding for the gradient,

$$\begin{array}{ccc} \mathrm{H}^1(\Omega) & \xrightarrow{\nabla} & [\mathrm{L}^2(\Omega)]^d \\ {\scriptstyle \pi_1}\big\downarrow & & \big\downarrow{\scriptstyle \pi_2} \\ X_h & \xrightarrow{\nabla_h} & \left[\mathbb{R}^d\right]^{\#\mathcal{T}} \end{array}$$

and this diagram moreover is commutative thanks to the formula $\int_K \nabla u \mathrm{d}x = \int_{\partial K} u \mathbf{n} \mathrm{d}l$, with $\mathbf{n}$ the unit normal on ∂K pointing outwards K.

2.3 Discrete variational embeddings

Definition 7. We consider a Lagrangian functional $\mathcal{L} :\ X \to \mathbb{R}$ as defined in definition 1 for some functional space $X \subset \mathrm{H}^1(\Omega)$. A discrete variational embedding is a discrete embedding $\mathcal{L}_h$ of $\mathcal{L}$ as defined in definition 4 in the particular framework $Y = \mathbb{R} = Y_h$ and $\pi_2 = id$. The diagram for a discrete variational embedding is the following,

$$\begin{tikzcd} X \arrow[r, "\mathcal{L}"] \arrow[d, "\pi_1"'] & \mathbb{R} \\ X_h \arrow[ur, "\mathcal{L}_h"'] & \end{tikzcd}$$

Finite element discrete variational embedding

We consider a general Lagrangian functional $\mathcal{L}$ as in definition 1. We use here the same framework as in section 2.2.2. The mesh is assumed to be simplicial. We consider $X = C^1(\Omega)$, $X_h = P^1(\mathcal{T})$ and the projection $\pi_1 : \ u \in C^1(\Omega) \mapsto \pi_1 u = (u_S)_{S\in\mathcal{N}} \in X_h$ with $u_S = u(S)$. Since $P^1(\mathcal{T}) \subset \mathrm{H}^1(\Omega)$ we define $\mathcal{L}_h : \ P^1(\mathcal{T}) \to \mathbb{R}$ as $\mathcal{L}_h = \mathcal{L}_{|P^1(\mathcal{T})}$. We have the diagram,

$$\begin{tikzcd} C^1(\Omega) \arrow[r, "\mathcal{L}"] \arrow[d, "\pi_1"'] & \mathbb{R} \\ P^1(\mathcal{T}) \arrow[ur, "\mathcal{L}_h"'] & \end{tikzcd}$$

Note that this definition extends to any conformal finite element space X_h, since we always have $X_h \subset \mathrm{H}^1(\Omega)$ (see e.g.[3, 14]). Of course the definition of π_1 needs to be adapted to each particular choice of X_h.
Also note that the extension to non-conforming finite elements is possible since $\mathcal{L}$ can be evaluated on any function u that would only be locally H^1, over each cell of the mesh (precisely $u_{|K} \in \mathrm{H}^1(K)$ for all $K \in \mathcal{T}$) instead than globally H^1 on the whole domain Ω.

2.4 Coherence

Consider a problem associated with a Lagrangian variational structure and consider this problem either under its variational formulation (Lagrangian least action principle),

$$\text{find} \quad u \in M \subset X \quad \text{so that} \quad \forall\, v \in V, \quad D\mathcal{L}(u)(v) = 0, \tag{12}$$

or under its differential formulation (Euler-Lagrange equation),

$$\text{find} \quad u \in M' \subset X' \quad \text{so that} \quad P(u) = 0, \tag{13}$$

where $P(u)$ defined in equation (3) is the operator associated to the Euler-Lagrange equation.
Under the conditions of theorem 1, these two formulations are equivalent. They however give rise to two discretisation procedures.

– Being given $\mathcal{L}_h$ a discrete variational embedding of $\mathcal{L}$ as in definition 7, the discrete least action principle reads

$$\text{find} \quad u_h \in M_h \subset X_h \quad \text{so that} \quad \forall\, v_h \in V_h, \quad D\mathcal{L}_h(u_h)(v_h) = 0. \tag{14}$$

This is a discrete variational formulation.

– Being given a discrete differential embedding of P as in definition 5,

$$\text{find} \quad u_h \in M'_h \subset X'_h \quad \text{so that} \quad P_h(u_h) = 0. \tag{15}$$

This is a discrete differential formulation.

A priori, the two discrete problems (14) and (15) do not provide equivalent problems. This question is addressed considering the concept of *coherence* introduced in [5].

Definition 8 (Coherence)**.** Consider a Lagrangian functional $\mathcal{L}$ satisfying the hypothesis of theorem 1. The operator associated to its Euler Lagrange equation (2) is denoted P.
Consider a discrete variational embedding of $\mathcal{L}$ as in definition 7. It is associated to a functional $\mathcal{L}_h$ and to a discrete least action principle given by equation (14). Consider a discrete differential embedding of P as in definition 5: it is associated to an operator P_h. These embeddings are said coherent if the discrete variational formulation (14) and the discrete differential formulation (15) are equivalent (*i.e.* have the same solutions).
In other words the following diagram is commutative,

$$\begin{tikzcd}
u \mapsto \mathcal{L}(u) \arrow[r, "\text{disc. var. emb.}"] \arrow[d, "\text{L.A.P.}"'] & u_h \mapsto \mathcal{L}_h(u_h) \arrow[d, "\text{disc. L.A.P.}"] \\
u \text{ solution of PDE (13)} \arrow[r, "\text{disc. diff. emb.}"] & u_h \text{ solution of PDE}_h \text{ (15)} \\
\text{E.L. equation} & \text{disc. E.L. equation}
\end{tikzcd}$$

where L.A.P. stands for least action principle and E.L. for Euler Lagrange.

A general raised question then is: can we find conditions ensuring the coherence between the discrete differential and variational embeddings ?
In the next two parts we study the coherence for discrete differential embeddings of problems having a Lagrangian or Hamiltonian variational formulation. It turns out that one cannot set apart the coherence from the algebraic properties of P_h inherited from the one of P. More precisely a property of integration by parts type is required at the discrete level to ensure coherence.
A deeper insight into this relationship is gained by considering the Poisson problem. Assume one performs a discrete differential embedding Δ_h for the Laplacian. In all forthcoming examples, coherence is obtained in case Δ_h is the composition of a discrete gradient and a discrete divergence $\Delta_h = \mathrm{div}_h \circ \nabla_h$, and if in addition these two discrete operators fulfil a duality property of type Green-Gauss formula. This is the case for finite differences with formula (18), for finite volumes with formula (21) and for mimetic finite differences in section 4.3.

Coherence for conforming finite elements

We first consider the Poisson problem (4). As developed in section 1.2, this PDE is the Euler Lagrange equation associated with a least action principle on the Lagrangian functional $\mathcal{L}(u) = \int_\Omega \big(\frac{1}{2}|\nabla u|^2 - fu\big)\mathrm{d}x$ given in equation (5).
Let $X_h \subset \mathrm{H}^1_0(\Omega)$ be some conforming finite element space. We can define $\mathcal{L}_h = \mathcal{L}_{|X_h}$. This provides a discrete variational embedding of $\mathcal{L}$ as in definition 7. The numerical problem solved in practice is the linear problem $P_h(u_h) = 0$ on X_h (involving the mass and stiffness matrices) where the operator P_h is defined by,

$$\forall v_h \in X_h, \quad \int_\Omega P_h(u_h) v_h \mathrm{d}x = \int_\Omega \left(\nabla u_h \cdot \nabla v_h - f v_h\right) \, \mathrm{d}x = D\mathcal{L}_h(u_h)(v_h).$$

The operator P_h on X_h provides a discrete differential embedding for the operator $P(u) = -\Delta u - f$ but is not explicit. By construction, these two discrete variational and differential embeddings are coherent.

The coherence for conforming finite element methods naturally extends to the PDE $P(u) = 0$ in equation (2) for an homogeneous Dirichlet boundary condition. This problem derives from a least action principle associated with the Lagrangian functional $\mathcal{L}$ in definition 1. On one hand we have a discrete variational embedding with $\mathcal{L}_h = \mathcal{L}_{|X_h}$. On the other hand the problem solved in practice is $P_h(u_h) = 0$ with $P_h(u_h)$ defined as,

$$\forall\, v_h \in X_h, \quad \int_\Omega P_h(u_h)\, v_h \,\mathrm{d}x = \int_\Omega \Big(\frac{\partial L}{\partial y}(x, u_h, \nabla u_h)\, v_h + \frac{\partial L}{\partial z}(x, u_h, \nabla u_h)\cdot \nabla v_h\Big)\, \mathrm{d}x,$$

that provides a discrete differential embedding of P. These discrete embeddings are coherent by construction.

3 Coherence of classical discrete embeddings

In section 2.4, we showed a first example of coherent discrete embedding of Lagrangian structure. In this precise case, several facilities were available: the discrete solution also is a function $u_h : \ \Omega \to \mathbb{R}$ so that differentiation and integration had the same sense at the discrete and at the continuous levels. As a result the definition of a discrete Lagrangian $\mathcal{L}_h$ was obvious and natural: $\mathcal{L}_h$ was the restriction of $\mathcal{L}$ to some functional space of finite dimension.
Such facilities are not always available, they rather are restricted to conforming finite element methods. Such a lifting between the discrete space of unknowns X_h and a function space is not available in general. As a result differentiation and integration have to be re-defined at the discrete level to provide a definition of a discrete Lagrangian. In this section we give two examples of discrete embeddings for a Lagrangian structure: finite differences and classical finite volumes. Coherence is proved in both cases.

3.1 Finite differences

We refer to [22] for a general presentation of finite difference methods. We study in this section the coherence properties of finite difference methods applied firstly to the Poisson problem (4) and secondly to the general Euler-Lagrange PDE (2). The domain is set to $\Omega = [0,1]^2$. We consider a Cartesian grid $\mathcal{T}$ of Ω with uniform size $h = 1/N$, $N \in \mathbb{N}^*$, in every direction. The results of this section can be extended to more general domains, to other space dimensions and more general lattices.
We will use the following notations. For $\mathbf{j} = (i,j) \in \mathbb{Z}^2$ we write $0 \le \mathbf{j} \le N$ if $0 \le i \le N$ and $0 \le j \le N$. Let $J = \{\mathbf{j} \in \mathbb{N}^2,\ 0 \le \mathbf{j} \le N\}$. The point of coordinates $(ih, jh) \in \overline{\Omega}$ is denoted $x_{\mathbf{j}}$. The mesh with vertexes $\{x_{\mathbf{j}},\ \mathbf{j} \in J\}$ is denoted $\mathcal{T}$, it is a cartesian grid of Ω.
Let us consider the two spaces $\mathcal{S} = \{u :\ \mathbb{Z}^2 \longrightarrow \mathbb{R}\}$ and $\mathcal{V} = \{\mathbf{p} :\ \mathbb{Z}^2 \longrightarrow \mathbb{R}^2\}$. Let $\mathbf{j} = (i,j) \in \mathbb{Z}^2$: we denote for $u \in \mathcal{S}$, $u_{i,j} = u_{\mathbf{j}} = u(\mathbf{j})$ and for $\mathbf{p} \in \mathcal{V}$, $\mathbf{p}_{i,j} = \mathbf{p}_{\mathbf{j}} = \mathbf{p}(\mathbf{j})$. We consider the discrete space

$$X_h = \{u \in \mathcal{S},\ u_{\mathbf{j}} = 0 \ \text{ if } \ \mathbf{j} \notin J \ \text{ and if } \ x_{\mathbf{j}} \in \partial\Omega\}.$$

The truncation operator $T :\ \mathcal{S} \to X_h$ is defined as $\big(Tu\big)_{\mathbf{j}} = u_{\mathbf{j}}$ if $0 < \mathbf{j} < N$ and by $\big(Tu\big)_{\mathbf{j}} = 0$ otherwise.

3.1.1 Discrete differential embedding for the Laplacian

The discrete Laplacian $\Delta_h :\ \mathcal{S} \to \mathcal{S}$ is defined as, for $\mathbf{j} = (i,j) \in \mathbb{Z}^2$,

$$(\Delta_h u)_{\mathbf{j}} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h^2}.$$

The operator $T \circ \Delta_h :\ \mathcal{S} \to X_h$ induces a mapping on X_h. Considering the projection $\pi_1 :\ C^0(\Omega) \to X_h$, given by $(\pi_1 u)_{\mathbf{j}} = u(x_{\mathbf{j}})$ if $0 < \mathbf{j} < N$, or $(\pi_1 u)_{\mathbf{j}} = 0$ otherwise, we have the following discrete differential embedding:

$$\begin{array}{ccc}
C^2(\Omega) & \xrightarrow{\Delta} & C^0(\Omega) \\
{\scriptstyle \pi_1}\big\downarrow & & \big\downarrow{\scriptstyle \pi_1} \\
X_h & \xrightarrow{T\circ\Delta_h} & X_h
\end{array}$$

For $f \in C^0(\Omega)$, the discrete differential embedding of $P(u) = -\Delta u - f$ then is $P_h(u_h) = -T \circ \Delta_h u_h - \pi_1 f$ for $u_h \in X_h$. The discrete differential formulation of the Poisson problem is,

$$\text{find} \quad u \in X_h \quad \text{so that} \quad P_h(u) = -T \circ \Delta_h u - \pi_1 f = 0. \tag{16}$$

Let us introduce a discrete gradient $\nabla_h :\ \mathcal{S} \to \mathcal{V}$ and a discrete divergence $\mathrm{div}_h :\ \mathcal{V} \to \mathcal{S}$. For $\mathbf{j} = (i,j) \in \mathbb{Z}^2$ they are given by,

$$(\nabla_h u)_{\mathbf{j}} = \frac{1}{h}\begin{pmatrix} u_{i+1,j} - u_{i,j} \\ u_{i,j+1} - u_{i,j} \end{pmatrix}, \quad (\mathrm{div}_h\, \mathbf{p})_{\mathbf{j}} = \frac{p^1_{i,j} - p^1_{i-1,j}}{h} + \frac{p^2_{i,j} - p^2_{i,j-1}}{h},$$

for $u \in \mathcal{S}$ and $\mathbf{p} = (p^1, p^2) \in \mathcal{V}$ ($p^1 \in \mathcal{S}$ and $p^2 \in \mathcal{S}$ are the two components of $\mathbf{p}$). This defines two discrete differential embeddings,

$$\begin{array}{ccc} C^1(\Omega) & \xrightarrow{\nabla} & [C^0(\Omega)]^2 \\ {\scriptstyle \pi_1}\big\downarrow & & \big\downarrow{\scriptstyle \pi_2} \\ X_h & \xrightarrow{T_2 \circ \nabla_h} & X_h \times X_h \end{array} \quad , \qquad \begin{array}{ccc} [C^1(\Omega)]^2 & \xrightarrow{\mathrm{div}} & C^0(\Omega) \\ {\scriptstyle \pi_2}\big\downarrow & & \big\downarrow{\scriptstyle \pi_1} \\ X_h \times X_h & \xrightarrow{T \circ \mathrm{div}_h} & X_h \end{array}$$

with $\pi_2 = \pi_1 \times \pi_1$ and $T_2 = T \times T$ component by component.
As one can see, a forward finite difference formula has been used for the definition of the discrete gradient, whereas a backward one has been used for the discrete divergence. This choice has been made in order to have the following properties (that can easily be checked). We have the composition rule,

$$\Delta_h = \mathrm{div}_h \circ \nabla_h, \tag{17}$$

and the *discrete Green-Gauss formula*:

$$\forall\, u \in X_h, \quad \forall\, \mathbf{p} \in \mathcal{V}: \quad \sum_{\mathbf{j} \in J} \mathbf{p}_{\mathbf{j}} \cdot (\nabla_h u)_{\mathbf{j}} = -\sum_{\mathbf{j} \in J} (\mathrm{div}_h\, \mathbf{p})_{\mathbf{j}}\; u_{\mathbf{j}}. \tag{18}$$

3.1.2 Discrete variational embedding, coherence

For $f \in C^0(\Omega)$ we introduce the discrete Lagrangian functional:

$$\forall\, u \in X_h, \quad \mathcal{L}_h(u) = \frac{1}{2} \sum_{\mathbf{j} \in J} |\nabla_{\mathbf{j}} u|^2\; h^2 \; - \; \sum_{\mathbf{j} \in J} (\pi_1 f)_{\mathbf{j}} u_{\mathbf{j}}\; h^2.$$

This definition provides the following discrete variational embedding for the Poisson Lagrangian functional $\mathcal{L}: \; u \mapsto \int_\Omega (\frac{1}{2}|\nabla u|^2 - fu)\mathrm{d}x$ given in equation (5),

$$\begin{tikzcd} C^1(\Omega) \arrow[r, "\mathcal{L}"] \arrow[d, "\pi_1"'] & \mathbb{R} \\ X_h \arrow[ur, "\mathcal{L}_h"'] & \end{tikzcd}$$

The discrete variational formulation of the Poisson problem reads:

$$\text{find}\, u \in X_h \quad \text{so that} \quad \forall\, v_h \in X_h: \quad D\mathcal{L}_h(u)(v_h) = 0. \tag{19}$$

Theorem 2. The discrete variational and differential embeddings of the Poisson problem using the finite difference method are coherent. Precisely, the two discrete problems (16) and (19) have the same solutions.

Proof. Let us consider a solution u to (19). We have for all $v_h \in X_h$,

$$\sum_{\mathbf{j} \in J} (\nabla_h u)_{\mathbf{j}} \cdot (\nabla_h v_h)_{\mathbf{j}}\; h^2 - \sum_{\mathbf{j} \in J} (\pi_1 f)_{\mathbf{j}} v_{\mathbf{j}}\; h^2 = 0.$$

Using the discrete Green-Gauss formula (18), we get: for all $v_h \in X_h$,

$$-\sum_{\mathbf{j}\in J} \left(\mathrm{div}_h(\nabla_h u)\right)_{\mathbf{j}} \; v_{\mathbf{j}} \; h^2 - \sum_{\mathbf{j}\in J} (\pi_1 f)_{\mathbf{j}} v_{\mathbf{j}} \; h^2 = 0.$$

Using the composition rule (17), this exactly means, for all $\mathbf{j}$ so that $0 < \mathbf{j} < N$, $-\left(\Delta_h u\right)_{\mathbf{j}} = (\pi_1 f)_{\mathbf{j}}$, which is equation (16). $\square$

3.1.3 Extension

The previous coherence theorem extends to the general Euler-Lagrange PDE (2) that we recall,

$$P(u) = \frac{\partial L}{\partial y}(x, u(x), \nabla u(x)) - \mathrm{div}\left(\frac{\partial L}{\partial z}(x, u(x), \nabla u(x))\right) = 0.$$

This equation is considered here together with a homogeneous boundary condition on $\partial\Omega$. The two discrete differential embeddings for the gradient and for the divergence introduced in section 3.1.1 provide the following discrete differential embedding $P_h : \; X_h \to X_h$. It is defined for $u \in X_h$ by,

$$\forall\, \mathbf{j} \in \mathbb{Z}^2, \quad (P_h u)_{\mathbf{j}} = \frac{\partial L}{\partial y}\left(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u)_{\mathbf{j}}\right) - \left(\mathrm{div}_h\, \mathbf{q}\right)_{\mathbf{j}} = 0$$
$$\text{with} \quad \mathbf{q} \in \mathcal{V}, \quad \mathbf{q}_{\mathbf{j}} = \frac{\partial L}{\partial z}(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u)_{\mathbf{j}}) \quad \forall\, \mathbf{j} \in \mathbb{Z}^2.$$

The differential form for the discretisation of the PDE (2) is,

$$\text{find} \quad u \in X_h \quad \text{such that} \quad P_h(u) = 0.$$

We can define the discrete Lagrangian $\mathcal{L}_h : \; X_h \longrightarrow \mathbb{R}$ for $u \in X_h$ by,

$$\forall\, \mathbf{j} \in \mathbb{Z}^2, \quad \left(\mathcal{L}_h u\right)_{\mathbf{j}} = \sum_{\mathbf{j}\in J} L\big(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u)_{\mathbf{j}}\big) \; h^2 \,.$$

It provides a discrete variational embedding for $\mathcal{L}$. The associated discrete variational formulation of the problem is:

$$\text{find}\, u \in X_h \quad \text{such that} \qquad D\mathcal{L}_h(u)(v) = 0 \quad \text{for any} \;\; v \in X_h.$$

We conserve in this framework the coherence result enunciated in theorem 2. It is similarly the consequence of the discrete Green-Gauss formula (18). Precisely a solution to the discrete variational formulation of the problem satisfies for all $v \in X_h$,

$$\sum_{\mathbf{j}\in J} \frac{\partial L}{\partial y}\left(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u)_{\mathbf{j}}\right) v_{\mathbf{j}} \; h^2 + \sum_{\mathbf{j}\in J} \frac{\partial L}{\partial z}\left(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u)_{\mathbf{j}}\right) \cdot (\nabla_h v)_{\mathbf{j}} \; h^2 = 0.$$

With the discrete Green-Gauss formula (18) we get:

$$\sum_{\mathbf{j}\in J} \left(\frac{\partial L}{\partial y}(x_{\mathbf{j}}, u_{\mathbf{j}}, \nabla_{\mathbf{j}} u) - (\mathrm{div}_h\, \mathbf{q})_{\mathbf{j}}\right) v_{\mathbf{j}} \; h^2 = 0$$

and we exactly recover the discrete differential formulation of the problem.

3.2 Finite Volumes

We focus in this section on the classical finite volume method (as presented *e.g.* in [10]) for the Poisson problem (4). We consider a mesh $\mathcal{T}$ of the domain Ω as in definition 6. Relatively to this mesh we assume that we can build two sets of points: cell centres $(x_K)_{K\in\mathcal{T}}$ and boundary face centres $(x_e)_{e\in\mathcal{E}_0}$ that satisfy:

$$\begin{aligned} \forall\ K \in \mathcal{T}, \quad \forall\ e \in \mathcal{E}_0 : &\quad x_K \in K,\ x_e \in e. \\ \forall\ e \in \mathcal{E}_i : &\quad e = K_1|K_2,\ [x_{K_1}, x_{K_2}] \perp e, \\ \forall\ e \in \mathcal{E}_0 : &\quad e = K|\partial\Omega,\ [x_e, x_K] \perp e. \end{aligned}$$

These two conditions are referred to as *admissibility* conditions. They impose a strong constraint on the mesh $\mathcal{T}$. Distances $(d_e)_{e\in\mathcal{E}}$ across the faces are defined as follows:

$$\begin{aligned} \forall\ e = K_1|K_2 \in \mathcal{E}_i : d_e = |x_{K_1}x_{K_2}|, \\ \forall\ e = K|\partial\Omega \in \mathcal{E}_0 : d_e = |x_K x_e|. \end{aligned}$$

3.2.1 Discrete differential embedding

We consider the settings in section 2.2.1: $X = [\mathrm{H}^1(\Omega)]^d$, $Y = \mathrm{L}^2(\Omega)$, $X_h = \mathbb{R}^{\#\mathcal{E}}$ and $Y_h = \mathbb{R}^{\#\mathcal{T}}$. We recall that the projections $\pi_1 :\ X \to X_h$ and $\pi_2 :\ Y \to Y_h$ are the normal component mean values on the mesh faces and the mean values on the mesh cells respectively.
The finite volume divergence $\mathrm{div}_h :\ Y_h \to X_h$ is defined in equation (9) that we recall,

$$\mathrm{div}_K\, \mathbf{p}_h = \frac{1}{|K|} \sum_{e\in\mathcal{E}, e\subset\partial K} p_e|e|\ \mathbf{n}_e \cdot \mathbf{n}_{K,e},$$

with the same notation $\mathrm{div}_K\, \mathbf{p}_h := (\mathrm{div}_h\, \mathbf{p}_h)_K$.

The flux operator $\mathcal{F} :\ \mathrm{H}^2(\Omega) \to \mathbb{R}^{\#\mathcal{E}}$ (thus relatively to the mesh $\mathcal{T}$) is defined as $\mathcal{F} = \pi_1 \circ \nabla$ (it consists in averaging the gradient of a function over the edges in their normal direction). The discrete flux operator is defined as:

$$\mathcal{F}_h :\ u_h = (u_K)_{K\in\mathcal{T}} \in \mathbb{R}^{\#\mathcal{T}} \mapsto (\mathcal{F}_e u_h)_{e\in\mathcal{E}} \in \mathbb{R}^{\#\mathcal{E}},$$

with,

$$\begin{aligned} \forall\ e = K_1|K_2 \in \mathcal{E}_i \ &:\ \mathcal{F}_e u_h = \frac{u_{K_2} - u_{K_1}}{d_e} \mathbf{n}_{K_1,e} \cdot \mathbf{n}_e, \\ \forall\ e = K|\partial\Omega \in \mathcal{E}_0 \ &:\ \mathcal{F}_e u_h = -\frac{u_K}{d_e} \mathbf{n}_{K,e} \cdot \mathbf{n}_e. \end{aligned}$$

Numerical fluxes across edges (and according to their intrinsic orientation) thus are computed using a finite difference scheme. Note that the Dirichlet boundary condition has implicitly being taken into account when defining the numerical fluxes on the boundary faces. This provides a discrete embedding for the flux operator $\mathcal{F}$:

$$\begin{tikzcd} \mathrm{H}^2(\Omega) \arrow[r, "\mathcal{F}"] \arrow[d, "\pi_3"'] & \mathbb{R}^{\#\mathcal{E}} \\ \mathbb{R}^{\#\mathcal{T}} \arrow[ur, "\mathcal{F}_h"'] & \end{tikzcd}$$

where the projection π_3 is defined as $(\pi_3 u)_K = u(x_K)$, *i.e.* as the values of the function u at each cell centre x_K.

The discrete Laplace operator Δ_h is defined as,

$$\Delta_h : \ \mathbb{R}^{\#\mathcal{T}} \to \mathbb{R}^{\#\mathcal{T}}, \quad \Delta_h = \mathrm{div}_h \circ \mathcal{F}_h.$$

For $f \in \mathrm{L}^2(\Omega)$, the discrete differential embedding of $P(u) = -\Delta u - f$ then is $P_h(u_h) = -\Delta_h u_h - \pi_2 f$ for $u_h \in \mathbb{R}^{\#\mathcal{T}}$. The differential formulation for the discrete Poisson problem is,

$$\text{find } u_h \in \mathbb{R}^{\#\mathcal{T}} \quad \text{so that} \quad P_h(u_h) = -\Delta_h u_h - \pi_2 f = 0. \tag{20}$$

Moreover we have the following *discrete Green-Gauss formula*: for all $p = (p_e)_{e\in\mathcal{E}} \in \mathbb{R}^{\#\mathcal{E}}$ and for all $u_h = (u_K)_{K\in\mathcal{T}} \in \mathbb{R}^{\#\mathcal{T}}$,

$$\sum_{K\in\mathcal{T}} (\mathrm{div}_K\, p)\, u_K |K| = -\sum_{e\in\mathcal{E}} p_e \mathcal{F}_e u_h |e| d_e. \tag{21}$$

3.2.2 Discrete variational embedding, coherence

In the continuous case, the diffusion energy $\int_\Omega |\nabla u|^2/2\,\mathrm{d}x$ is part of the Lagrangian functional $\mathcal{L}$. In the framework of finite volume method, no proper *discrete gradient* is available, but only numerical fluxes in the normal direction to the mesh faces. Thus only the normal component (and not the tangential one) of some *discrete gradient* on the mesh faces is approximated.
We recall that $\pi_2 f = (f_K)_{K\in\mathcal{T}}$ with $f_K = \int_K f\,\mathrm{d}x/|K|$, see section 2.2.1. We introduce the discrete Lagrangian functional $\mathcal{L}_h : \ \mathbb{R}^{\#\mathcal{T}} \to \mathbb{R}$ as

$$\mathcal{L}_h(u_h) = \frac{1}{2}\sum_{e\in\mathcal{E}} (\mathcal{F}_e u_h)^2 \ |e| d_e \ - \sum_{K\in\mathcal{T}} f_K u_K \ |K|.$$

The functional $\mathcal{L}_h$ defines a discrete variational embedding of $\mathcal{L}$. The variational form for the finite volume discrete Poisson problem is,

$$\text{find} \quad u_h \in \mathbb{R}^{\#\mathcal{T}} \quad \text{such that} \quad \forall\, v_h \in \mathbb{R}^{\#\mathcal{T}}, \quad D\mathcal{L}_h(u_h)(v_h) = 0. \tag{22}$$

Theorem 3. The discrete variational and differential embeddings of the Poisson problem using the finite volume method are coherent. Precisely, the discrete differential formulation (20) and discrete variational formulation (22) for the Poisson problem have the same solutions.

Proof. Let u_h satisfy (22), we have by differentiating $\mathcal{L}_h$: for all $u_h, v_h \in \mathbb{R}^{\#\mathcal{T}}$,

$$D\mathcal{L}_h(u_h)(v_h) = \sum_{e\in\mathcal{E}} \big(\mathcal{F}_e u_h\big)\big(\mathcal{F}_e v_h\big)|e|d_e \; - \; \sum_{K\in\mathcal{T}} (\pi_2 f)_K v_K |K| = 0.$$

Using the discrete Green-Gauss formula (21), we get for all $u_h, v_h \in \mathbb{R}^{\#\mathcal{T}}$,:

$$-\sum_{K\in\mathcal{T}} \left(\mathrm{div}_K(\mathcal{F}_h u_h)\right) v_K |K| - \sum_{K\in\mathcal{T}} (\pi_2 f)_K v_K |K| = 0,$$

which is equivalent with (20). □

4 Hamiltonian calculus of variations and mixed formulations

In this section let L be an admissible Lagrangian function as defined in section 1.1. We recall the link between Hamiltonian and Lagrangian systems in section 4.1. We will stress here the relationships between mixed formulations and discrete embedding of Hamiltonian systems in section 4.3.

4.1 Hamiltonian formulation

Definition 9 (Legendre property)**.** We say that L satisfies the Legendre property if the mapping $z \mapsto \dfrac{\partial L}{\partial z}(x, y, z)$ is a bijection on $\mathbb{R}^d$ for any $x \in \Omega$ and any $y \in \mathbb{R}$.

If L satisfies the Legendre property, the following function $g : \Omega\times\mathbb{R}\times\mathbb{R}^d \to \mathbb{R}^d$ is well defined:

$$z = g(x, y, \mathbf{p}) \quad \text{with} \quad \mathbf{p} = \frac{\partial L}{\partial z}(x, y, z).$$

Let us consider $\mathbf{p} = \dfrac{\partial L}{\partial z}(x, y, z)$ as a new variable, then,

$$\mathbf{p} = \frac{\partial L}{\partial z}\big(x, y, g(x, y, \mathbf{p})\big) \quad \text{and} \quad g\big(x, y, \frac{\partial L}{\partial z}(x, y, z)\big) = z\,.$$

Definition 10 (Hamiltonian)**.** Let L satisfy the Legendre property. The Hamiltonian $H : \Omega \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ associated to L is:

$$H(x, y, \mathbf{p}) = \mathbf{p} \cdot g(x, y, \mathbf{p}) - L(x, y, g(x, y, \mathbf{p})).$$

We introduce two different definitions for the Hamiltonian functional $\mathcal{H} :\ \mathrm{Dom}(\mathcal{H}) \subset \mathrm{L}^2(\Omega) \times \left[\mathrm{L}^2(\Omega)\right]^d \to \mathbb{R}$ associated to H:

1. Primal Hamiltonian, $\mathrm{Dom}(\mathcal{H}) = \mathrm{H}^1(\Omega) \times [\mathrm{L}^2(\Omega)]^d$,
$$\mathcal{H}(u, \mathbf{p}) = \int_\Omega \mathbf{p} \cdot \nabla u - H(x, u, \mathbf{p})\, \mathrm{d}x. \tag{23}$$

2. Dual Hamiltonian, $\mathrm{Dom}(\mathcal{H}) = \mathrm{L}^2(\Omega) \times \mathrm{H}_{\mathrm{div}}(\Omega)$,
$$\mathcal{H}(u, \mathbf{p}) = \int_\Omega - \mathrm{div}(\mathbf{p}) u - H(x, u, \mathbf{p})\, \mathrm{d}x. \tag{24}$$

Proposition 2. According to definition 2, the Hamiltonian functional $\mathcal{H}$ is differentiable at point $(u, \mathbf{p}) \in \mathrm{Dom}(\mathcal{H})$ if
$$\frac{\partial H}{\partial y}(x, u, \mathbf{p}) \in \mathrm{L}^2(\Omega) \quad \text{and} \quad \frac{\partial H}{\partial \mathbf{p}}(x, u, \mathbf{p}) \in \left[\mathrm{L}^2(\Omega)\right]^d.$$

In such a case we have, for $(v, \mathbf{q}) \in \mathrm{Dom}(\mathcal{H})$:

- In the primal case:
$$D\mathcal{H}(u, \mathbf{p})\cdot(v, \mathbf{q}) = \int_\Omega \left[\mathbf{q} \cdot \left(\nabla u - \frac{\partial H}{\partial \mathbf{p}}(x, u, \mathbf{p})\right) + \nabla v \cdot \mathbf{p} - v\frac{\partial H}{\partial y}(x, u, \mathbf{p})\right] \mathrm{d}x. \tag{25}$$

- In the dual case:
$$D\mathcal{H}(u, \mathbf{p})\cdot(v, \mathbf{q}) = \int_\Omega \left[- \mathrm{div}(\mathbf{q}) u - \mathbf{q} \cdot \frac{\partial H}{\partial \mathbf{p}}(x, u, \mathbf{p}) - v\left(\mathrm{div}\, \mathbf{p} + \frac{\partial H}{\partial y}(x, u, \mathbf{p})\right)\right] \mathrm{d}x.$$

Definition 11 (Extremals)**.** Let us consider a space of variation $V \times W \subset \mathrm{Dom}(\mathcal{H})$. We say that $(u, \mathbf{p}) \in \mathrm{Dom}(\mathcal{H})$ is an extremal for $\mathcal{H}$ relatively to $V \times W$ if $\mathcal{H}$ is differentiable at point $(u, \mathbf{p})$ and:
$$\forall\ (v, \mathbf{q}) \in V \times W, \quad D\mathcal{H}(u, \mathbf{p}) \cdot (v, \mathbf{q}) = 0.$$

Theorem 4 (Hamilton's least action principle)**.** Let $(u, \mathbf{p}) \in \mathrm{Dom}(\mathcal{H})$ be an extremal for $\mathcal{H}$ relatively to $V \times W$. Assume moreover that:

- in the primal case: $\mathbf{p} \in \mathrm{H}_{\mathrm{div}}(\Omega)$, $V_0 = \{v \in V, v = 0 \text{ on } \partial\Omega\}$ is dense in $\mathrm{L}^2(\Omega)$ and W is dense in $[\mathrm{L}^2(\Omega)]^d$,
- in the dual case: $u \in \mathrm{H}^1(\Omega)$, V is dense in $\mathrm{L}^2(\Omega)$ and $W_0 = \{\mathbf{q} \in W, \mathbf{q} \cdot n = 0 \text{ on } \partial\Omega\}$ is dense in $[\mathrm{L}^2(\Omega)]^d$.

Then $(u, \mathbf{p})$ is a solution of the *Hamiltonian system*:
$$\left\{\begin{array}{ll} \mathrm{div}\, \mathbf{p} & = -\dfrac{\partial H}{\partial y}(x, u, \mathbf{p}) \\ \nabla u & = \dfrac{\partial H}{\partial \mathbf{p}}(x, u, \mathbf{p}). \end{array}\right. \tag{26}$$

Proof. Let us consider the case of the primal definition of the Hamiltonian functional $\mathcal{H}$. Since $\mathbf{p} \in \mathrm{H}_{\mathrm{div}}(\Omega)$, using the Green formula in (25) gives: $\forall\ (v, \mathbf{q}) \in V \times W$,

$$\int_\Omega \Big(-\big(\operatorname{div} \mathbf{p} + \frac{\partial H}{\partial y}(x, u, \mathbf{p})\big)\, v + \mathbf{q} \cdot \big(\nabla u - \frac{\partial H}{\partial \mathbf{p}}(x, u, \mathbf{p})\big) \Big) \mathrm{d}x \ + \int_{\partial\Omega} v\ \mathbf{p} \cdot \mathbf{n}\, ds = 0.$$

The boundary integral vanishes for $v \in V_0$. We recover (26) by density of V_0 in $\mathrm{L}^2(\Omega)$ and of W in $[\mathrm{L}^2(\Omega)]^d$. □

Corollary 1 (Lagrangian and Hamiltonian formulations)**.** The solutions $(u, \mathbf{p})$ of the Hamiltonian system (26) are exactly the solutions of the Euler-Lagrange equation (2) under the condition

$$\mathbf{p} = \frac{\partial L}{\partial z}(x, u, \nabla u).$$

Application to the Poisson problem

We consider the Poisson problem (4). We recall that the Lagrangian function associated with this problem is

$$L(x, y, z) = \frac{1}{2} z \cdot z - f(x) y.$$

The Legendre property is clearly satisfied by L. We introduce the new variable $\mathbf{p} = z$ and the function g is given by $g(x, y, \mathbf{p}) = \mathbf{p}$. A Hamiltonian for the Poisson problem is then given by,

$$H(x, y, \mathbf{p}) = \mathbf{p} \cdot \mathbf{p} - L(x, y, g(x, y, \mathbf{p})) = \frac{1}{2} \mathbf{p} \cdot \mathbf{p} + f(x) y. \tag{27}$$

The Hamiltonian system (26) associated with (27) is the mixed formulation of the Poisson problem (4):

$$\begin{cases} -\operatorname{div} \mathbf{p} & = f \\ \nabla u & = \mathbf{p}\,. \end{cases} \tag{28}$$

Applying theorem 4, one obtains that the weak solutions of the Poisson problem in its mixed form (28) exactly are extremals for the Hamiltonian functional $\mathcal{H}$ in (27). Precisely:

- Primal form (23) of $\mathcal{H}$. Consider an extremal $(u, \mathbf{p}) \in \mathrm{H}^1_0(\Omega) \times [\mathrm{L}^2(\Omega)]^d$ of $\mathcal{H}$ relatively to the space of variations $V \times W = \mathrm{H}^1_0(\Omega) \times [\mathrm{L}^2(\Omega)]^d$. An extremal exactly is a solution for the primal weak formulation of the mixed Poisson equation: find $(u, \mathbf{p}) \ \in \mathrm{H}^1_0(\Omega) \times [\mathrm{L}^2(\Omega)]^d$ such that,

$$\begin{cases} -\int_\Omega \mathbf{p} \cdot \nabla v \ \mathrm{d}x = -\int_\Omega f v \ \mathrm{d}x & \forall\ v \in \mathrm{H}^1_0(\Omega) \\ \int_\Omega (\mathbf{p} - \nabla u) \cdot \mathbf{q} \ \mathrm{d}x = 0 & \forall\ \mathbf{q} \in [\mathrm{L}^2(\Omega)]^d\ . \end{cases}$$

- Dual form (24) of $\mathcal{H}$. Consider an extremal $(u, \mathbf{p}) \in \mathrm{L}^2(\Omega) \times \mathrm{H}_{\mathrm{div}}(\Omega)$ of $\mathcal{H}$ relatively to the space of variations $V \times W = \mathrm{L}^2(\Omega) \times \mathrm{H}_{\mathrm{div}}(\Omega)$. An extremal exactly is a solution for the dual weak formulation of the mixed Poisson equation that reads: find $(u, \mathbf{p}) \in \mathrm{L}^2(\Omega) \times \mathrm{H}_{\mathrm{div}}(\Omega)$ such that

$$\begin{cases} \int_\Omega (\operatorname{div} \mathbf{p} + f) v \, \mathrm{d}x = 0 & \forall\, v \in \mathrm{L}^2(\Omega) \\ \int_\Omega \mathbf{p} \cdot \mathbf{q} \, \mathrm{d}x + \int_\Omega u \operatorname{div} \mathbf{q} \, \mathrm{d}x = 0 & \forall\, \mathbf{q} \in \mathrm{H}_{\mathrm{div}}(\Omega) \,. \end{cases}$$

4.2 Coherence

The definition of the discrete differential embedding in section 2 applies to the Hamiltonian system where P is given by

$$P(u, \mathbf{p}) = \begin{pmatrix} \operatorname{div} \mathbf{p} + \dfrac{\partial H}{\partial y}(x, u, \mathbf{p}) \\ \nabla u - \dfrac{\partial H}{\partial \mathbf{p}}(x, u, \mathbf{p}) \end{pmatrix} .$$

The definition 7 of the discrete variational embedding also applies to Hamiltonian system by replacing $\mathcal{L}$ by $\mathcal{H}$. The definition of coherence for the discretisation of Hamiltonian systems is the same as definition 8 for Lagrangian systems.

Definition 12. Let us consider a discrete differential embedding of the mixed problem (26). If the discrete problem solutions exactly are extremals of a discrete Hamiltonian functional $\mathcal{H}_h$ that moreover also is a discrete variational embedding of $\mathcal{H}$, then we say that we have coherence.
In case of coherence we then have the following commutative diagram:

$$\begin{array}{ccc} (u, \mathbf{p}) \mapsto \mathcal{H}(u, \mathbf{p}) & \xrightarrow{\text{disc. var. emb.}} & (u_h, \mathbf{p}_h) \mapsto \mathcal{H}_h(u_h, \mathbf{p}_h) \\ \text{L.A.P.} \downarrow & & \downarrow \text{disc. L.A.P.} \\ (u, \mathbf{p}) \quad \text{solution of PDE (26)} & \xrightarrow{\text{disc. diff. emb.}} & (u_h, \mathbf{p}_h) \quad \text{solution of the discrete PDE} \\ \text{Hamiltonian system} & & \text{disc. Hamiltonian system} \end{array}$$

where L.A.P. stands for least action principle.

Remark 2. In section 2.4 it was shown that the coherence for conforming finite element naturally derives from the method definition. The same conclusion also holds for conforming mixed finite elements. The discrete Hamiltonian in that case is the restriction of the Hamiltonian $\mathcal{H}$ to the finite element space.

4.3 Mimetic Finite Differences

We consider the mixed formulation (28) of the Poisson problem together with a homogeneous Dirichlet condition $u = 0$ on $\partial\Omega$. The scalar products on

$L^2(\Omega)$ and on $[L^2(\Omega)]^d$ are respectively denoted, for u, $v \in L^2(\Omega)$ and for $\mathbf{p}$, $\mathbf{q} \in [L^2(\Omega)]^d$,

$$(u, v) = \int_\Omega uv \; \mathrm{d}x, \quad [\mathbf{p}, \mathbf{q}] = \int_\Omega \mathbf{p} \cdot \mathbf{q} \; \mathrm{d}x.$$

The Green-Gauss formula rewrites as, for all $u \in H^1_0(\Omega)$ and all $\mathbf{p} \in H_{\mathrm{div}}(\Omega)$,

$$[\mathbf{p}, \nabla u] = -(\operatorname{div} \mathbf{p}, u).$$

In the Mimetic Finite Differences (MFD) framework, a discrete flux operator $\mathcal{F}_h : Y_h \to X_h$ is defined as (minus) the adjoint of the finite volume discrete divergence (see section 2.2.1) after the introduction of a scalar product on X_h that is consistent with $[\cdot, \cdot]$. We refer to [2] for the MFD discretisation of diffusion problems.

4.3.1 Discrete differential embedding

A mesh $\mathcal{T}$ of the domain Ω is considered as in definition 6. The space $P^0(\mathcal{T})$ of the piecewise constant functions over the mesh cells is considered and identified with $\mathbb{R}^{\#\mathcal{T}}$. Since $P^0(\mathcal{T}) \subset L^2(\Omega)$, the L^2 scalar product on $P^0(\mathcal{T})$ is available.
The notations in section 2.2.1 for the finite volume divergence are considered: $X_h = \mathbb{R}^{\#\mathcal{E}}$ and $\pi_1 : [H^1(\Omega)]^d \to X_h$, $\pi_2 : L^2(\Omega) \to P^0(\mathcal{T})$ are the projections in the diagram (10). We adopt the following alternative (but equivalent) definition for the finite volume divergence in the diagram (10). We introduce the space $\tilde{X}_h$:

$$\begin{aligned} \tilde{X}_h = \{p_{K,e} \quad & \text{for} \quad K \in \mathcal{T} \quad \text{and for} \quad e \in \mathcal{E} \quad \text{so that} \quad e \subset \partial K \\ & \text{that satisfy} \quad p_{K_1,e} + p_{K_2,e} = 0 \quad \text{if} \quad e = K_1 | K_2\}. \end{aligned}$$

An element $\mathbf{p} \in \tilde{X}_h$ is given by one numerical flux on each external face and by two opposite numerical fluxes per internal face. Obviously, $\tilde{X}_h$ is isomorphic to X_h. With this identification we get the new commutative diagram for the discrete divergence,

$$\begin{array}{ccc} [H^1(\Omega)]^d & \xrightarrow{\operatorname{div}} & L^2(\Omega) \\ {\scriptstyle \tilde{\pi}_1}\big\downarrow & & \big\downarrow{\scriptstyle \pi_2} \\ \tilde{X}_h & \xrightarrow{\operatorname{div}_h} & P^0(\mathcal{T}) \end{array}$$

where $\tilde{\pi}_1$ is given by $\tilde{\pi}_1 \mathbf{p} = (p_{K,e})$ with $p_{K,e} = \int_e \mathbf{p} \cdot \mathbf{n}_{K,e} \mathrm{d}l / |e|$ the mean flux of $\mathbf{p}$ across the face e according to the unit normal to e pointing outwards K. The discrete divergence within this framework has the following expression (to be compared to (9)), $\operatorname{div}_h : \mathbf{p} = (p_{K,e}) \in \tilde{X}_h \mapsto (\operatorname{div}_K \mathbf{p})_{K \in \mathcal{T}} \in P^0(\mathcal{T})$:

$$\operatorname{div}_K \mathbf{p} = \frac{1}{|K|} \sum_{e \in \mathcal{E}, e \subset \partial K} p_{K,e} |e|.$$

The definition of a scalar product on $\tilde{X}_h$ is not obvious. Let us consider $K \in \mathcal{T}$ and denote $\tilde{X}_h^K$ the restriction of $\tilde{X}_h$ to K. We suppose that a cell scalar product $[\cdot,\cdot]_K$ is given on each $\tilde{X}_h^K \in \mathcal{T}$ and that the scalar product on $\tilde{X}_h$ decomposes as:

$$\forall\ \mathbf{p}_h, \mathbf{q}_h \in \tilde{X}_h : \quad [\mathbf{p}_h, \mathbf{q}_h]_h = \sum_{K\in\mathcal{T}} [\mathbf{p}_h, \mathbf{q}_h]_K, \tag{29}$$

A way to define the elemental scalar product (29) is to introduce a lifting operator $\mathcal{R}_K : \tilde{X}_h^K \longrightarrow [\mathrm{L}^2(K)]^d$ and then to define:

$$[\mathbf{p}_h, \mathbf{q}_h]_K = \int_K \mathcal{R}_K(\mathbf{p}_h) \cdot \mathcal{R}_K(\mathbf{q}_h) \mathrm{d}x. \tag{30}$$

For more details on the construction of $\mathcal{R}_K$, we refer to [2]. The present definitions are sufficient for our purpose. Relatively to the scalar product (29), the discrete flux operator $\mathcal{F}_h : P^0(\mathcal{T}) \longrightarrow \tilde{X}_h$ is defined as (minus) the adjoint of the discrete divergence: $\mathcal{F}_h = -\operatorname{div}_h^\star$. It is uniquely determined by,

$$\forall\ u_h,\ \mathbf{p}_h \in P^0(\mathcal{T}) \times \tilde{X}_h : \quad [\mathbf{p}_h, \mathcal{F}_h u_h]_h = -(\operatorname{div}_h \mathbf{p}_h, u_h).$$

The discrete differential embedding for the mixed Poisson problem (28) using the MFD method then is defined by $P_h :\ P^0(\mathcal{T}) \times \tilde{X}_h \to P^0(\mathcal{T}) \times \tilde{X}_h$:

$$P_h(u_h, \mathbf{p}_h) = \begin{pmatrix} -\operatorname{div}_h \mathbf{p}_h - \pi_2 f \\ \mathbf{p}_h - \mathcal{F}_h u_h \end{pmatrix}.$$

The discretisation of the mixed Poisson problem (28) is : find $u_h \in P^0(\mathcal{T})$ and $\mathbf{p}_h \in \tilde{X}_h$ such that,

$$P_h(u_h, \mathbf{p}_h) = 0. \tag{31}$$

4.3.2 Discrete variational embedding, coherence

The Hamiltonian H for the Poisson problem is given in equation (27). The associated Hamiltonian functional $\mathcal{H}$ with the primal definition (23), $\mathrm{Dom}(\mathcal{H}) = \mathrm{H}^1(\Omega) \times [\mathrm{L}^2(\Omega)]^d$,

$$\begin{aligned}\mathcal{H}(u, \mathbf{p}) &= \int_\Omega \mathbf{p} \cdot \nabla u \,\mathrm{d}x - \frac{1}{2}\int_\Omega \mathbf{p}\cdot\mathbf{p}\,\mathrm{d}x - \int_\Omega f u \,\mathrm{d}x \\ &= [\mathbf{p}, \nabla u] - \frac{1}{2}[\mathbf{p},\mathbf{p}] - (u, f)\,.\end{aligned}$$

We therefore define the discrete Hamiltonian $\mathcal{H}_h :\ P^0(\mathcal{T}) \times \tilde{X}_h \to \mathbb{R}$ as,

$$\mathcal{H}_h(u_h, \mathbf{p}_h) = [\mathbf{p}_h, \mathcal{F}_h u_h]_h - \frac{1}{2}[\mathbf{p}_h, \mathbf{p}_h]_h - (u_h, \pi_2 f)_h\,.$$

It provides the following discrete variational embedding,

$$\begin{tikzcd} \mathrm{H}^1_0(\Omega) \times [\mathrm{H}^1(\Omega)]^d \arrow[r, "\mathcal{H}"] \arrow[d, "\pi_2\times\tilde{\pi}_1"'] & \mathbb{R} \\ P^0(\mathcal{T}) \times \tilde{X}_h \arrow[ur, "\mathcal{H}_h"'] & \end{tikzcd}$$

The variational form for the MFD discrete mixed Poisson problem is: find $(u_h, \mathbf{p}_h) \in P^0(\mathcal{T}) \times \tilde{X}_h$ such that,

$$\forall\ (v_h, \mathbf{q}_h) \in P^0(\mathcal{T}) \times \tilde{X}_h, \quad D\mathcal{H}_h(u_h, \mathbf{p}_h)(v_h, \mathbf{q}_h) = 0. \tag{32}$$

Theorem 5. The MFD discrete differential formulation (31) and variational formulation (32) for the mixed Poisson problem are equivalent. Then the MFD discretisation for the mixed Poisson problem is coherent.

Proof. Differentiating $\mathcal{H}_h$ gives:

$$D\mathcal{H}_h(u_h, \mathbf{p}_h)(v_h, \mathbf{q}_h) = [\mathbf{p}_h, \mathcal{F}_h v_h]_h + [\mathcal{F}_h u_h, \mathbf{q}_h]_h - [\mathbf{p}_h, \mathbf{q}_h]_h - (\pi_2 f, v_h)_h\,.$$

Using that $\mathcal{F}_h = -\operatorname{div}_h^\star$ relatively to the scalar product $[\cdot,\cdot]_h$ we obtain,

$$D\mathcal{H}_h(u_h, \mathbf{p}_h)(v_h, \mathbf{q}_h) = (-\operatorname{div}_h \mathbf{p}_h - \pi_2 f, v_h)_h + [\mathcal{F}_h u_h - \mathbf{p}_h, \mathbf{q}_h]_h\,.$$

Therefore singular points for $\mathcal{H}_h$ exactly are the solutions to equation (31). $\square$

5 Conclusion

In the present paper we studied the properties of the discretisation of PDEs deriving from a variational principle, either Lagrangian or Hamiltonian. We addressed the following questions. Does the discrete problem also satisfy a variational principle ? If it does, what is the relationship between that variational principle and the one that rules the PDE ? These questions are analysed by introducing the concepts of discrete variational and discrete differential embeddings and of coherence between these two types of embeddings.
For the Poisson problem, considering several classical methods, we showed that the discrete Poisson equation is associated to a variational embedding. A crucial property ensuring coherence for the discrete problems is the following. The Euler Lagrange PDE involves two differential operators of order one: a gradient and a divergence. The differential embeddings of these two operators must satisfy some duality property. That property is a discrete analogous of the Green-Gauss formula.

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