COHERENT DISCRETE EMBEDDINGS FOR LAGRANGIAN AND HAMILTONIAN SYSTEMS

by

J. Cresson, I. Greff & C. Pierre

Abstract. — The general topic of the present paper is to study the conservation for some structural property of a given problem when discretising this problem. Precisely we are interested with Lagrangian or Hamiltonian structures and thus with variational problems attached to a least action principle. Considering a partial differential equation (PDE) deriving from such a variational principle, a natural question is to know whether this structure at the continuous level 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. In case 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 (finite elements, finite differences and finite volumes). Hamiltonian structures are shown to provide coherence between a discrete Hamiltonian structure and the discretisation of the mixed formulation of the PDE, both for mixed finite elements and mimetic finite differences methods.

Contents

Key words and phrases. — Lagrangian systems, Hamiltonian systems, variational integrators, discrete embeddings, numerical schemes, FEM, FVM, DFM, mixed formulation, mimetic.

Introduction

Many problems arising in various fields (such as physics, mechanics, fluid mechanics or finance) are described using partial differential equations (PDEs). Although explicit solutions are not available in general, important classes of PDEs do present strong structural properties: classical examples are symmetry properties, maximum principle or conservation properties. It is quite essential for the numerical methods to provide a translation of these structural properties from the continuous level to the discrete level so enforcing the numerical solutions to obey qualitative behaviours in agreement with the underlying physic 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 informations 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). A range of numerical methods forget about the Lagrangian to focus on the Euler-Lagrange equation itself. This is for example the case for the finite difference methods.

In this paper we address the first following question: *consider a PDE deriving from a Lagrangian and a least action principle. When discretising this PDE, how is embedded the attached Lagrangian structure at the discrete level ?* More precisely we ask whether the discretised PDE can be seen as deriving from a *discrete least action principle* associated with a *discrete Lagrangian* structure. Basically, in case the Lagrangian structure is embedded at the discrete level, then the variational property of the original equation (at the continuous level) may be preserved by the discrete problem.

Aside from the Lagrangian systems are the Hamiltonian systems: under suitable conditions a Lagrangian system can be reformulated as a Hamiltonian one. PDEs deriving from an Hamiltonian structure inherit strong properties such as energy conservation or existence of first integrals. Such PDEs moreover concern a wide class of problems: like mixed formulations and saddle point problems [**3**] that usually are associated with an important class of numerical methods (mixed finite elements e.g.).

The second question we address in this paper is whether Hamiltonian structures can be embedded at the discrete level: *do numerical solutions of PDEs deriving from a Hamiltonian structure also derive from a discrete Hamiltonian structure ?* Again, in case a Hamiltonian structure is embedded at the discrete level, strong and interesting properties might be inherited by the numerical solutions.

The concept of *coherence* is introduced to answer these two questions. Let us consider a problem having a Lagrangian structure. That is to say consider a Lagrangian functional $\mathcal{L}$ on a functional space and the attached calculus of variations. The solutions to the continuous problem satisfy a least action principle that reads a second order PDE: the Euler-Lagrange equation. Discretisation can be performed at two different levels:

- either discretise the Euler-Lagrange equation by defining discrete analogues to the differential operators in this PDE. We will call *discrete differential embedding* this procedure,
- or discretise the Lagrangian structure by defining a discrete Lagrangian functional $\mathcal{L}_h$. This second procedure is called *discrete variational embedding*. A calculus of variations then can be developed at the discrete level on $\mathcal{L}_h$ to define a discrete least action principle. This process of obtaining a discrete counterpart of the Euler-Lagrange equation with the help of the discretisation of the Lagrangian functional and the discrete least action principle is also called *variational integrator*. There is a wide range of work by Lubich [**17**], the group of Marsden [**18**] on this topic preserving structures for ODEs.

In case the two discrete differential and discrete variational embeddings do define equivalent discrete problems we will say that we have *coherence*. This is enunciated in saying that the following diagram commutates:

$$
\begin{array}{ccc}
\text{Lagrangian } \mathcal{L} & \xrightarrow{\text{disc. diff. emb.}} & \text{discrete Lagrangian } \mathcal{L}_h \\
{\scriptstyle \text{L.A.P.}}\big\downarrow & & \big\downarrow{\scriptstyle \text{disc. L.A.P.}} \\
\text{Euler-Lagrange equation} & \xrightarrow{\text{disc. var. emb.}} & \text{discrete Euler-Lagrange equation}
\end{array}
$$

where L.A.P stands for least-action principle. The same notion of coherence can be defined relatively to Hamiltonian structures.

In case of coherence, the discretisation firstly preserves the variational structure of the problem so inheriting interesting properties (such as independence with the coordinate system). It secondly may also preserves algebraic properties from the differential operators within the Euler-Lagrange equation.

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 classical problem being well documented both at the continuous and at the discrete levels, it provides an appropriate test case to improve the understanding of discrete embeddings for Lagrangian/Hamiltonian structures and of the embedding of variational properties from the continuous to the discrete level. Let us point out that such structures are not available for every common problems, such as convection problems or the Navier-Stokes equations. The structural numerical difficulties (numerical diffusion, stabilisation e.g.) attached to these problems have to be linked to this lack of variational structure. A general alternative to build new numerical schemes (or variational integrators) for such problems would be:

1. construct a non classical variational structure for the considered problem as in [**8, 9, 10**],
2. embed this structure at the discrete level.

Although this paper is mainly concerned with improving the understanding of discrete embeddings of variational structures on a classical example, it is aimed to help towards the development of new numerical schemes for it helps in controlling the second step above.

The outline of the paper is as follows. Part I gives an informal introduction to embedding formalism. We introduce the notions of discrete differential and discrete variational embeddings of a given problem, as well as the concept of coherence between these two embeddings.

Part II deals with Lagrangian systems. In section 4 are defined the Lagrangian structure and the associated calculus of variations for fields. The Lagrangian structure for the Poisson equation is recalled in section 5. In section 6 is presented the discrete embedding of a Lagrangian structure: the principle of coherence is defined and conforming finite element methods are here shown to satisfy the coherence principle for general Euler-Lagrange PDEs.

In part III we focus on the Poisson equation and on the coherence of two classical numerical methods for this problem: finite differences and finite volumes in sections 7 and 8 respectively.

Part IV is concerned with Hamiltonian structures and mixed formulations. Hamiltonian structure and the associated calculus of variations are presented in section 9. One recover the mixed form of the Poisson problem through its Hamiltonian formulation. The discrete embedding of Hamiltonian structure and the notion of coherent embedding are presented in section 10: coherence is shown to be naturally fulfilled by conforming mixed finite element methods. Coherence of mimetic finite difference methods, [**4**], for the mixed Poisson problem is analysed in the last section.

The general notations are detailed and listed at the end of the paper.

PART I
DISCRETE EMBEDDINGS

The formalism of embeddings has been initiated in [**8**] and further developed in [**6**], [**9**], [**11**], [**2**]. This part introduces, on an informal way, the notion of discrete embeddings in the case of partial differential equations. The definitions will be detailed in parts II, III and IV. For a complete introduction to embedding formalisms for PDEs we refer to [**7**].

1. Discrete differential embeddings

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and let M denotes some functional space on Ω. In general, a PDE can be written as: find $u \in M$ so that,

$$P(u) = 0, \tag{1}$$

where P is a differential operator. This differential operator can be written in different forms. As an example, the classical Laplacian operator

$$\Delta = \sum_{i=1}^{d} \partial_{x_i}^2,$$

can be rewritten as

$$\Delta = \operatorname{div} \circ \nabla.$$

We will adopt the following informal definition of a discrete differential embedding of PDE (1):

Definition 1 **(Discrete differential embedding)**. — *A discrete differential embedding of equation (1) is formally obtained by: firstly providing a discrete space M_h (of finite dimension) in which the discrete solution u_h will be sought and secondly by providing a discrete operator P_h on M_h analogue to P.*
The discrete differential embedding of equation (1) becomes: find $u_h \in M_h$ so that

$$P_h(u_h) = 0. \tag{2}$$

As an example, let us formally consider Δ_h, div_h and ∇_h discrete analogues of the operators Δ, div and ∇ (precisions being given in the sequel). This leads to two discrete differential embeddings for the Poisson problem: find $u_h \in M_h$ so that either,

$$\Delta_h u_h = 0,$$

or,

$$\operatorname{div}_h(\nabla_h u_h) = 0.$$

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.
A second problem related to discrete differential embeddings is that it is based on the form of the operator P, which form depends on the considered coordinate system (used to write the equation).

2. Discrete variational embeddings

We here assume that equation (1) derives from a variational principle. Precisely that it is obtained from a least action principle on a functional

$$\mathcal{L} : M \to \mathbb{R},$$

namely, that the solutions of equation (1) coincide with the critical points of $\mathcal{L}$. Being considered a subset $V \subset M$ referred to as the *set of variations* and denoting $D\mathcal{L}(u)(v)$ the Gâteau derivative of $\mathcal{L}$ along a direction $v \in V$, we precisely have: for any $u \in M$:

$$P(u) = 0 \quad \Leftrightarrow \quad D\mathcal{L}(u)(v) = 0\,, \ \forall\ v \in V.$$

This is referred to as a *variational formulation* for problem (1) and the correspondence between the solutions of the PDE and the critical points of the functional a *variational principle*.

Rather than discretising the differential operator P (i.e. to perform a discrete differential embedding as previously defined) we here are led to the following alternative: discretise the functional $\mathcal{L}$ and define the discrete solutions u_h through a variational principle on $\mathcal{L}_h$.

***Definition 2* (Discrete variational embedding).** — *Assume that the PDE (1) has a variational formulation given by a functional $\mathcal{L}$ and a set of variations $V \subset M$. A discrete variational embedding of equation (1) is formally obtained by: firstly providing a discrete space M_h (of finite dimension) and a discrete set of variations $V_h \subset M_h$ and secondly by defining a discrete functional $\mathcal{L}_h : M_h \to \mathbb{R}$ analogue of $\mathcal{L}$.*
The variational embedding of equation (1) is then defined as: find $u_h \in M_h$ such that

$$D\mathcal{L}_h(u_h)(v_h) = 0, \quad \forall\ v_h \in V_h, \tag{3}$$

(i.e. u_h is a critical point of $\mathcal{L}_h$ for the variation set V_h).

Discrete variational embeddings essentially possess interesting properties. The main one being that the underlying object supporting the discretisation does not depend on the coordinate system, on the contrary of the differential form (1) of the problem and therefore of its discrete differential embedding. Discrete variational embedding corresponds to the so-called variational integrators studied for ODEs by Lubich [**17**] and the group of Marsden [**18**].

3. Coherence of differential and variational embeddings

As formally introduced here, there is no reason for the two discrete differential and variational embeddings of a given problem to provide equivalent discrete problems. This question is addressed considering the concept of *coherence* introduced in [**8**]. An informal statement is the following :

***Definition 3* (Coherence).** — *Let problem* (1) *have a variational formulation. Two given discrete differential and variational embeddings for* (1) *are said to be in coherence in case the two discrete problems* (2) *and* (3) *are equivalent.*

In case of coherence, the discretisation of problem (1) not only preserves its variational structure but also the algebraic one of P.

A general raised question then is: Can we find conditions ensuring the coherence between the discrete differential and variational embeddings ?

In the next three parts we study the coherence for discrete 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 for properties of integration by part type. A deeper insight into this relationship is gained by considering the Poisson problem. When performing a discrete differential embedding for the Poisson problem involving both a discrete gradient and a discrete divergence (to define P_h), coherence is obtained in case these two discrete operators fulfil some discrete analogue of the Green-Gauss formula. This is the case for finite differences with formula (11) as detailed in remark 4. This also is the case for finite volumes with formula (22) in remark 5. Considering the mimetic finite difference (see section 11 in part IV), such a discrete Green-Gauss formula is a priori imposed in order to build the scheme and coherence here again is satisfied.

PART II
DISCRETE VARIATIONAL EMBEDDING OF LAGRANGIAN SYSTEMS

In the first section, we recall classical results about Lagrangian calculus of variations. Section 5 deals with the Lagrangian formulation of the Poisson problem. The notions of discrete variational embedding and coherence in the Lagrangian case are specified in section 6. As a first example, we discuss the case of conforming finite element methods.

4. Lagrangian calculus of variations

In this section we define basics on calculus of variations applied to vector fields. For more details, we refer to the books of Evans [**12**], Giaquinta and Hildebrand [**14**], [**15**]. Let us note $M = L^2(\Omega)$.

Definition 4. — *An admissible Lagrangian function L is a continuous function*

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

such that L is of class $\mathcal{C}^2$ with respect to y and v. Let us consider a subspace $\mathrm{Dom}(\mathcal{L})$ *of $H^1(\Omega)$ satisfying: for all $u \in \mathrm{Dom}(\mathcal{L})$, $L(\cdot, u(\cdot), \nabla u(\cdot)) \in L^1(\Omega)$. The Lagrangian function L defines the Lagrangian functional $\mathcal{L}$:*

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

We are interested in vanishing the first variations of the Lagrangian functional $\mathcal{L}$ on a space of variations V. As in [**14**], we could give general notion of extremals and variations. We take the following definitions of the notions of differentiable functional and extremal for $\mathcal{L}$.

***Definition 5* (Differentiability).** — *We consider a space of variations* $V \subset \mathrm{Dom}(\mathcal{L})$. *The functional* $\mathcal{L}$ *is differentiable at point* $u \in \mathrm{Dom}(\mathcal{L})$ *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 $V = \mathrm{Dom}(\mathcal{L})$ and $D\mathcal{L}(u)$ is continuous on $\mathrm{Dom}(\mathcal{L})$. The definition given here suffices to introduce extremals:

***Definition 6* (Extremals).** — *A function* $u \in \mathrm{Dom}(\mathcal{L})$ *is an extremal for the functional* $\mathcal{L}$ *relatively to the space of variations* $V \subset \mathrm{Dom}(\mathcal{L})$ *if* $\mathcal{L}$ *is differentiable at point* u *and:*

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

***Proposition 1*.** — *The Lagrangian functional* $\mathcal{L}$ *is differentiable at point* $u \in \mathrm{Dom}(\mathcal{L})$ *if:* $x \mapsto \dfrac{\partial L}{\partial y}(x, u(x), \nabla u(x))$ *and* $x \mapsto \dfrac{\partial L}{\partial v}(x, u(x), \nabla u(x))$ *are in* M *and* M^d *respectively. In such a case the differential is given for any* $v \in \mathrm{Dom}(\mathcal{L})$ *by:*

$$D\mathcal{L}(u)(v) = \int_\Omega \left[\frac{\partial L}{\partial y}\big(x, u(x), \nabla u(x)\big)\ v + \frac{\partial L}{\partial v}\big(x, u(x), \nabla u(x)\big) \cdot \nabla v \right] dx. \tag{4}$$

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

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

Integrating over the domain Ω gives:

$$\mathcal{L}(u{+}\epsilon v) = \mathcal{L}(u) + \int_\Omega \epsilon\, v\, \frac{\partial L}{\partial y}(x,u(x),\nabla u(x))dx + \int_\Omega \big(\epsilon \nabla v\big)\cdot \frac{\partial L}{\partial v}(x,u(x),\nabla u(x))dx + o(\epsilon),$$

leading to (4). □

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

***Theorem 1* (Least action principle).** — *Let us assume the Lagrangian functional* $\mathcal{L}$ *is differentiable at point* $u \in \mathrm{Dom}(\mathcal{L})$ *and that* u *is an extremal for a given space of variations* V. *Assume moreover that* $\frac{\partial L}{\partial v}(\cdot, u(\cdot), \nabla u(\cdot)) \in H_{\mathrm{div}}(\Omega)$ *and that the subspace* $V_0 = \{v \in V, v = 0 \text{ on } \partial\Omega\}$ *is dense in* M. *Then* u *satisfies the generalised Euler-Lagrange equation:*

$$\frac{\partial L}{\partial y}(x, u(x), \nabla u(x)) - \mathrm{div}\left(\frac{\partial L}{\partial v}(x, u(x), \nabla u(x)) \right) = 0. \tag{5}$$

Proof. — Following (4) and using the Green formula gives: $\forall\, v \in V_0$,

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

which implies (5) by density of V_0 in M. □

5. Lagrangian structure for the Poisson problem

We consider the following Poisson problem on Ω for a homogeneous Dirichlet boundary condition: find a solution u to

$$\text{(6)} \qquad \begin{cases} -\Delta u &= f \quad \text{in} \quad \Omega, \\ u &= 0 \quad \text{on} \quad \partial\Omega. \end{cases}$$

For a data $f \in M$, the problem (6) has a unique solution $u \in H^2 \cap H^1_0(\Omega)$.
For a function $f \in M$, we consider the (admissible) Lagrangian function L:

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

The associated Lagrangian functional $\mathcal{L}$ is defined on $\mathrm{Dom}(\mathcal{L}) = \mathrm{H}^1(\Omega)$ by:

$$\mathcal{L}(u) = \int_\Omega \frac{1}{2}|\nabla u(x)|^2 - f(x)u(x)dx,$$

and is differentiable on $H^1(\Omega)$.

Theorem 2. — *The solution of the Poisson problem (6) is the extremal $u \in V$ for $\mathcal{L}$ with the space of variations $V = H^1_0(\Omega)$.*

***Remark 1* (Generalisation).** — *Consider the general elliptic problem:*

$$\text{(7)} \qquad \begin{cases} -\operatorname{div}(\alpha \nabla u) &= f \quad in \quad \Omega, \\ u &= 0 \quad on \quad \partial\Omega. \end{cases}$$

for the tensor $x \in \Omega \mapsto \alpha(x) \in \mathbb{R}^{d\times d}$ (strongly elliptic, positive, symmetric, and bounded). The solution of problem (7) is the extremal $u \in H^1_0(\Omega)$ of the Lagrangian functional $\mathcal{L}$ associated with

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

and for the space of variations $V = H^1_0(\Omega)$.

6. Coherence for discrete embeddings of Lagrangian structure

In this section, we suppose given a conformal mesh $\mathcal{T}_h$ of the domain Ω. A precise definition for a mesh (which is not needed here) is given in definition 11. To the functional spaces M and V are associate discrete counterparts M_h and V_h. We suppose given a discrete Lagrangian functional $\mathcal{L}_h$ defined on M_h.

Remark 2. — *A general definition for a discrete Lagrangian is not obvious and greatly differs from a numerical scheme to another. In the following, we show that a discrete Lagrangian for the general Euler-Lagrange equation* (5) *is available in the case of conforming finite element methods. Part III deals with the definition of a* *discrete Lagrangian for the Poisson problem in the case of finite volume and finite difference methods.*

***Definition 7* (Discrete least action principle).** — *A discrete function $u_h \in M_h$ is an extremal of $\mathcal{L}_h$ relatively to a space of variations V_h if*

$$D\mathcal{L}_h(u_h)(v_h) = 0 \text{ for any } v_h \in V_h. \tag{8}$$

Equation (8) *is called the* **discrete Euler-Lagrange equation** *and the procedure* **discrete least action principle**.

***Definition 8* (Coherence principle).** — *A discretisation procedure is said coherent if the discrete differential embedding of the Euler-Lagrange equation* (5) *is the discrete Euler-Lagrange equation* (8) *coming from the discrete least action principle. This is equivalent to the commutation of the following diagram:*

$$\begin{array}{ccc}
u \in M \mapsto \mathcal{L}(u) & \xrightarrow{\text{disc. diff. emb.}} & u_h \in M_h \mapsto \mathcal{L}_h(u_h) \\
\text{L.A.P.}\downarrow & & \downarrow\text{disc. L.A.P.} \\
u \text{ solution of PDE} & \xrightarrow{\text{disc. var. emb.}} & u_h \text{ solution of } PDE_h \\
(\text{E.L. equation } (5)) & & (\text{discrete E.L. equation } (8))
\end{array}$$

In other words, the procedure is coherent if the direct discretisation of the Euler-Lagrange equation given by the discrete differential embedding leads to the same solutions as the one given by the associated discrete variational embedding.

Coherence for conforming finite element methods. — We consider here the Euler-Lagrange PDE (5) together with a homogeneous Dirichlet boundary condition $u = 0$ on $\partial\Omega$. For simplicity we assume that we can set $\mathrm{Dom}(\mathcal{L}) = \mathrm{H}^1_0(\Omega)$. We consider M_h a classical conforming finite element discretisation of $H^1_0(\Omega)$ relatively to the mesh $\mathcal{T}_h$. For instance, in case the mesh is a triangulation, M_h denotes the P^k-Lagrange finite element space of continuous functions polynomial of order k in each cell of the triangulation (see e.g.[**5, 16**]). We then define V_h as the subset of M_h made of the functions $u_h \in M_h$ that vanishes on $\partial\Omega$.

The discrete differential embedding of PDE (5) given by the finite element method is: find $u_h \in V_h$ such that, for all $v_h \in V_h$,

$$\int_\Omega \Big(\frac{\partial L}{\partial y}(x, u_h, \nabla u_h) v_h + \frac{\partial L}{\partial v}(x, u_h, \nabla u_h) \cdot \nabla v_h \Big) dx = 0. \tag{9}$$

A discrete variational embedding is provided by defining the discrete Lagrangian $\mathcal{L}_h$ as:

$$\mathcal{L}_h := \mathcal{L}_{|M_h}.$$

This definition holds since for conforming finite element methods $M_h \subset \mathrm{Dom}(\mathcal{L})$.

***Theorem 3* (Coherence).** — *The conforming finite element methods for PDE* (5) *is coherent. Precisely the singular points of the discrete Lagrangian $\mathcal{L}_h$ with respect to the space of variations V_h and the solutions of the discretisation* (9) *coincide.*

Remark 3. — *By definition conforming finite element methods are based on some weak formulation. This weak formulation might or might not be a variational formulation of some least action principle: this is typically the case for the Poisson equation but not for the for convection-diffusion or Navier-Stokes equation. If the* *weak formulation coincides with a variational formulation, the conforming finite element discretisation is naturally coherent with the underlying variational principle and the associated Lagrangian structure.*

PART III
COHERENCE OF CLASSICAL DISCRETE EMBEDDINGS

In section 6 of the previous part we showed a first example of coherent discrete embedding of Lagrangian structure. In this precise case, several facilities where available: the discrete solution had a clear definition as 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. In general, differentiation and integration have to be redefined at the discrete level to provide a definition of a discrete Lagrangian. In this part we give two examples of discrete embeddings for a Lagrangian structure: finite differences and classical finite volumes. Coherence is proved for the discretisation of the general Euler-Lagrange PDE (5) in the case of finite differences and in the case of the (isotropic) Poisson problem for finite volumes.

7. Finite differences

We consider in this section the general Euler-Lagrange PDE (5) together with a homogeneous Dirichlet boundary condition $u = 0$ on $\partial\Omega$. We refer to [**19**] concerning the finite difference method. For simplicity, the domain will here be set to $\Omega = [0,1]^d$. We consider a Cartesian grid $\mathcal{T}_h$ of Ω with uniform size $h = 1/N$, $N \in \mathbb{N}^*$, in each direction. The results of this section can be extended to more general domains and more general lattices without difficulty.

We will use the following notations here. For $\mathbf{j} = (j_1, \ldots, j_d) \in \mathbb{N}^d$, we denote $\mathbf{j}^{>i}$ (resp. $\mathbf{j}^{<i}$) the shift of $\mathbf{j}$ by $+1$ (resp -1) in the i^{th} component: $\mathbf{j}^{>i} := (j_1, \ldots, j_{i-1}, j_i{+}1, j_{i+1}, \ldots, j_d)$, J denotes the subset of $\mathbb{N}^d$ $J := \{\mathbf{j} \in \mathbb{N}^d,\ 0 \leq \mathbf{j} \leq N\}$. The point of coordinates $(j_1 h, \ldots, j_d h)$ is denoted $x_\mathbf{j} \in \mathbb{R}^d$. The considered grid $\mathcal{T}_h$ then is the grid with vertices $\{x_\mathbf{j},\ \mathbf{j} \in J\}$.

7.1. Discrete differential embedding. — Let us consider the two spaces of mappings: $\mathcal{S} := \{u_h:\ \mathbb{Z}^d \longrightarrow \mathbb{R}\}$ and $\mathcal{V} := \{\mathbf{F}_h:\ \mathbb{Z}^d \longrightarrow \mathbb{R}^d\}$, whose elements are respectively denoted $(u_\mathbf{j})$ and $(\mathbf{F}_\mathbf{j})$. We introduce the discrete gradient and discrete divergence operators: $\nabla_h:\ \mathcal{S} \longrightarrow \mathcal{V}$ and $\mathrm{div}_h:\ \mathcal{V} \longrightarrow \mathcal{S}$ as:

$$(10) \qquad (\nabla_h u_h)_\mathbf{j} = \frac{1}{h}\begin{pmatrix} u_{\mathbf{j}^{>1}} - u_\mathbf{j} \\ \vdots \\ u_{\mathbf{j}^{>d}} - u_\mathbf{j} \end{pmatrix}, \quad (\mathrm{div}_h\, \mathbf{F}_h)_\mathbf{j} = \sum_{i=1}^{d} \left[\frac{\mathbf{F}_\mathbf{j} - \mathbf{F}_{\mathbf{j}^{<i}}}{h}\right]_i,$$

where $[\mathbf{X}]_i$ stands for the i^{th} component of the vector $\mathbf{X} \in \mathbb{R}^d$.

We consider the discrete functional spaces M_h and V_h defined as: $M_h := \{u_h \in$

$\mathcal{S},\ u_{\mathbf{j}} = 0$ if $\mathbf{j} \notin J\}$ and $V_h := \{u_h \in M_h,\ u_{\mathbf{j}} = 0 \text{ if } \mathbf{j} \in \partial J\}$. The resort to $\mathcal{S}$ and $\mathcal{V}$ is motivated by the simplifications it provides in the notations only.

With these definitions, we have the following discrete Green-Gauss formula:

$$\forall\ u_h \in V_h,\ \forall\ \mathbf{F}_h \in \mathcal{V}: \quad \sum_{\mathbf{j}\in J} \mathbf{F}_{\mathbf{j}} \cdot (\nabla_h u_h)_{\mathbf{j}}\ h^d = -\sum_{\mathbf{j}\in J} (\mathrm{div}_h\, \mathbf{F}_h)_{\mathbf{j}}\ u_{\mathbf{j}}\ h^d. \tag{11}$$

Remark 4. — *Up to now, different choices have been made for the definition of discrete differentiation operators. The discrete gradient is defined using a forward Euler scheme whereas the discrete divergence uses a backward Euler differentiation formula. Other choices are possible: for instance forward on the divergence and backward on the gradient, or either a centered scheme for both operators. The crucial point is that whatever are their definitions, the two discrete operators have to commute in a discrete Green-Gauss formula of type* (11) *to eventually ensure the coherence.*

Definition 9. — *The discrete differential embedding given by the finite difference discretisation of the Euler-Lagrange PDE* (5) *reads: find $u_h \in V_h$ such that,*

$$\left(\frac{\partial L}{\partial y}(x, u_h, \nabla_h u_h) - \mathrm{div}_h \left(\frac{\partial L}{\partial v}(x, u_h, \nabla_h u_h) \right) \right)_{\mathbf{j}} = 0, \tag{12}$$

for all $\mathbf{j}$ such that $x_{\mathbf{j}} \in \Omega$ (i.e. $0 < \mathbf{j} < N$) and with:

$$\left(\frac{\partial L}{\partial y}(x, u_h, \nabla_h u_h) \right)_{\mathbf{j}} = \frac{\partial L}{\partial y}(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u_h)_{\mathbf{j}})$$
$$\left(\frac{\partial L}{\partial v}(x, u_h, \nabla_h u_h) \right)_{\mathbf{j}} = \frac{\partial L}{\partial v}(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u_h)_{\mathbf{j}})$$

7.2. Discrete variational embedding, coherence. —

***Definition 10* (Discrete Lagrangian)**. — *We consider the following definition for the discrete Lagrangian functional $\mathcal{L}_h :\ M_h \longrightarrow \mathbb{R}$, associated to the continuous Lagrangian functional $\mathcal{L} :\ M \longrightarrow \mathbb{R}$ given in definition 4*

$$\mathcal{L}_h(u_h) = \sum_{\mathbf{j}\in J} L(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u_h)_{\mathbf{j}})\ h^d. \tag{13}$$

The discrete Euler-Lagrange equation then is:

$$\text{Find } u_h \in V_h \text{ such that } : \quad D\mathcal{L}_h(u_h)(v_h) = 0 \quad \text{for any } \ v_h \in V_h. \tag{14}$$

***Theorem 4* (Coherence)**. — *The finite difference discretisation of the Euler-Lagrange PDE* (5) *is coherent in the sense with definition 8. Precisely: the solution of the discrete Euler-Lagrange equation* (14) *and the solution of the discretised Euler-Lagrange equation* (12) *coincide.*

Proof. — Let us consider a solution to (14). We then have:

$$\sum_{\mathbf{j}\in J} \frac{\partial L}{\partial y}(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u_h)_{\mathbf{j}}) v_{\mathbf{j}} + \sum_{\mathbf{j}\in J} \frac{\partial L}{\partial v}(x_{\mathbf{j}}, u_{\mathbf{j}}, (\nabla_h u_h)_{\mathbf{j}}) \cdot (\nabla_h v_h)_{\mathbf{j}} = 0.$$

Using the discrete Green-Gauss Formula (11) we exactly recover the discretised Euler-Lagrange equation (12). □

8. Finite Volumes

We consider in this section the classical finite volume method (as presented *e.g.* in [**13**]) for the Poisson problem (6). The following definitions and notations will be needed.

Definition 11 **(Mesh $\mathcal{T}_h$, cells K, faces $\mathcal{E}$ and vertices $\mathcal{N}$)**

A cell (or control volume), generically denoted K, is a polygonal/polyhedral open subset $K \subset \Omega$.
A mesh $\mathcal{T}_h$ of the domain Ω is a collection of cells K partitioning Ω in the following sense:

$$\cup_{K\in\mathcal{T}_h}\overline{K} = \overline{\Omega}\ ,\ \ K_1, K_2 \in \mathcal{T}_h\ \Rightarrow\ \text{either } K_1 \cap K_2 = \emptyset \text{ or } K_1 = K_2\ .$$

A face (or an edge) e of some $K \in \mathcal{T}_h$ 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 $K \in \mathcal{T}_h$ satisfying $e \subset \overline{K} \cap \partial\Omega$: one writes $e = K|\partial\Omega$.
The internal faces set $\mathcal{E}_i$ associated with $\mathcal{T}_h$ is the set of all geometrical subsets $e = \overline{K_1} \cap \overline{K_2}$, $K_1, K_2 \in \mathcal{T}_h$ and $K_1 \neq K_2$, having non-zero $(d-1)-$dimensional measure. For every $e \in \mathcal{E}_i$, there exist a unique couple $K_1, K_2 \in \mathcal{T}_h$ satisfying $e = \overline{K_1} \cap \overline{K_2}$: one writes $e = K_1|K_2$.
The faces set associated with $\mathcal{T}_h$ is given as $\mathcal{E} := \mathcal{E}_0 \cup \mathcal{E}_i$. It provides a partitioning of $\cup_{K\in\mathcal{T}_h}\partial K$, in the same meaning as earlier: $\cup_{e\in\mathcal{E}} e = \cup_{K\in\mathcal{T}_h}\partial K$ and the overlapping of two distinct faces either is empty or of zero $(d-2)-$dimensional measure.

Eventually, the set of vertices associated with $\mathcal{T}_h$ is denoted $\mathcal{N}$: it contains exactly all the vertices of all the cells $K \in \mathcal{T}_h$.

Let $e \in \mathcal{E}$ such that $e \subset \partial K$ for $K \in \mathcal{T}_h$. We denote $\mathbf{n}_{K,e}$ the unit normal to e pointing outward of K.

One shall also denote by $|O|$ 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 $e \in \mathcal{E}$ and $|xy|$ the length between two points x and y.

Two sets of points are introduced: cells centres $(x_K)_{K\in\mathcal{T}_h}$ and boundary faces centres $(x_e)_{e\in\mathcal{E}_0}$. They satisfy:

$$\forall\ K \in \mathcal{T}_h,\ \forall e \in \mathcal{E}_0 : x_K \in K,\ x_e \in e\ . \tag{15}$$

$$\forall e \in \mathcal{E}_i : e = K_1|K_2,\ [x_{K_1}, x_{K_2}] \perp e,$$
$$\forall e \in \mathcal{E}_0 : e = K|\partial\Omega,\ [x_e, x_K] \perp e. \tag{16}$$

Conditions (15)-(16) are referred to as *admissibility* conditions. They impose a strong constraint on the mesh $\mathcal{T}_h$. Non conformal meshes for instance cannot fulfil such a constraint.
Distances $(d_e)_{e\in\mathcal{E}}$ across the faces are defined as follows:

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

8.1. Discrete differential embedding. — To the mesh $\mathcal{T}_h$ is associated the discrete functional space M_h:

$$M_h := \{u_h \in M,\ u_h = \sum_{K\in\mathcal{T}_h} u_K \chi_K,\ u_K \in \mathbb{R}\}\ , \tag{17}$$

where χ_K is the characteristic function of the cell K: M_h is the space of piecewise constant functions on the cells $K \in \mathcal{T}_h$. An element $u_h \in M_h$ will be simply denoted by its component: $u_h = (u_K)_{K \in \mathcal{T}_h}$.

The following interpolation operator I is considered:

$$I : \ f \in M \mapsto f^I \in M_h \ , \quad f_K^I := \frac{1}{|K|} \int_K f \ dx \ , \quad \forall \ K \in \mathcal{T}_h. \tag{18}$$

To $u_h \in M_h$ are associated its *numerical fluxes* along the edges $e \in \mathcal{E}$, using a finite difference scheme as follows:

$$\begin{aligned} &\forall \ e = K_1|K_2 \in \mathcal{E}_i \ : \ F_{e,K_1} = \frac{u_{K_2} - u_{K_1}}{d_e}, \\ &\forall \ e = K|\partial\Omega \in \mathcal{E}_0 \ : \ F_{e,K} = -\frac{u_K}{d_e}. \end{aligned} \tag{19}$$

Definition (19) of the fluxes on the boundary is the discretisation of the homogeneous Dirichlet boundary condition in (6) considered here. Of particular importance is the following continuity relation:

$$\forall \ e = K_1|K_2 \in \mathcal{E}_i \ , \ F_{e,K_1} = -F_{e,K_2} \ . \tag{20}$$

This property motivates the following definition:

$$\forall \ e \in \mathcal{E} \ , \ F_e := |F_{e,K}| \ , \ \text{for any} \ \ K \in \mathcal{T}_h \text{ such that } \ e \subset \partial K \ .$$

Definition 12. — *A discrete Laplace operator $\Delta_h : \ M_h \to M_h$ is defined as follows. For $u_h \in M_h$:*

$$\forall K \in \mathcal{T}_h \ , \ (\Delta_h u_h)_K := \frac{1}{|K|} \sum_{e \in \mathcal{E}, \ e \subset \partial K} F_{e,K} |e| \ .$$

The discrete differential embedding given by the finite volume scheme for problem (6) *reads:*

$$\textit{find} \ \ u_h \in M_h \ \textit{so that} \ : \ -\Delta_h u_h \ = \ f^I \ . \tag{21}$$

Remark 5. — *It is interesting to consider the discrete Laplacian Δ_h as the composition of the flux operator in* (19) *with a discrete divergence operator (of finite volume type). Being given a flux distribution $F = (F_{e,K})_{e \in \mathcal{E}, \ e \in \partial K}$, the discrete divergence is given on each cell $K \in \mathcal{T}_h$ by:*

$$\operatorname{div}_K F = \frac{1}{|K|} \sum_{e \in \partial K} F_{e,K} |e|.$$

In this way Δ_h in definition 12 expresses a flux balance on each cell K mimicking in a discrete context the divergence formula.

Moreover we have the discrete Green-Gauss formula for a flux distribution F satisfying the continuity property (20) *and for $u_h \in M_h$:*

(22)

$$\sum_{K \in \mathcal{T}_h} (\operatorname{div}_K F) \, u_K |K| = - \sum_{e = K_1|K_2 \in \mathcal{E}_i} F_{e,K_1} \frac{u_{K_2} - u_{K_1}}{d_e} |d_e||e| + \sum_{e = K|\partial\Omega \in \mathcal{E}_0} F_{e,K} u_K |e|.$$

8.2. Discrete variational embedding, coherence. — In the continuous case, the energy term $|\nabla u|^2$ is part of the Lagrangian functional $\mathcal{L}$. In the framework of finite volume method, no proper *discrete gradient* is available. Actually the numerical fluxes definition (19) involves a discrete differentiation in the normal direction to the mesh faces. Thus only the normal component of some *discrete gradient* on the mesh faces is approximated in the finite volume framework and not the tangential one.
The discrete differentiation along the face normal direction is used to define a discrete Lagrangian functional:

Definition 13. — *The discrete Lagrangian functional $\mathcal{L}_h : M_h \to \mathbb{R}$ is defined as:*

$$\forall u_h \in M_h \ , \ \mathcal{L}_h(u_h) = \frac{1}{2} \sum_{e\in\mathcal{E}} F_e^2 \ |e| d_e \ - \sum_{K\in\mathcal{T}_h} f_K^I u_K \ |K| \ . \tag{23}$$

***Theorem 5* (Coherence).** — *The finite volume discretisation for the Poisson problem* (6) *is coherent in the sense of definition 8. Precisely: let us consider the discrete least action principle associated with* (23)*: find $u_h \in M_h$ such that,*

$$\forall \ v_h \in M_h \ : \quad D\mathcal{L}_h(u_h)(v_h) = 0.$$

Then this problem has a unique solution which is moreover the unique solution of (21)*.*
Note that here $M_h = V_h$, the boundary condition being encoded directly in the definition of the discrete Laplace operator (through the fluxes definition (19)*) and not in the choice of the variation space.*

Proof. — With definition (23), $\mathcal{L}_h$ is clearly strictly convex and has a unique minimum. Differentiating (23), it comes: $\forall \ u_h, v_h \in M_h$,

$$\begin{aligned} D\mathcal{L}_h(u_h)(v_h) = \ - \sum_{K\in\mathcal{T}_h} f_K^I v_K |K| \ + \sum_{e=K|\partial\Omega\in\mathcal{E}_0} \frac{u_K}{d_e} v_K |e| \\ + \sum_{e=K_1|K_2\in\mathcal{E}_i} \frac{u_{K_1} - u_{K_2}}{d_e} (v_{K_1} - v_{K_2}) |e| \ . \end{aligned}$$

Using the discrete Green-Gauss formula (22) with the flux distribution F equal to the flux of u_h given by (19) we simply get:

$$D\mathcal{L}_h(u_h)(v_h) = - \sum_{K\in\mathcal{T}_h} \left(f_K^I + \operatorname{div}_K F \right) v_K |K| \ = - \sum_{K\in\mathcal{T}_h} \left(f_K^I + (\Delta_h u_h)_K \right) v_K |K|.$$

Thus, the condition $D\mathcal{L}_h(u_h)(v_h) = 0$ for all $v_h \in M_h$ exactly reads $-\Delta_h u_h = f^I$. □

PART IV
HAMILTONIAN CALCULUS OF VARIATIONS AND MIXED FORMULATIONS

In this part let $L : \ \Omega \times \mathbb{R} \times \mathbb{R}^d$ be an admissible Lagrangian function as defined in section 4. We recall the link between Hamiltonian and Lagrangian systems.

Moreover we try to understand the mixed formulation as a Hamiltonian system. As an application, we consider the Poisson problem.
Let us recall that $M = L^2(\Omega)$ and $X = [L^2(\Omega)]^d$.

9. Hamiltonian and mixed formulation

9.1. Hamiltonian formulation. —

***Definition 14* (Legendre property).** — *We say that L satisfies the Legendre property if the mapping $v \mapsto \dfrac{\partial L}{\partial v}(x,y,v)$ is a bijection on $\mathbb{R}^d$ for any $x \in \Omega$, $y \in \mathbb{R}$.*

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:

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

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

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

***Definition 15* (Hamiltonian).** — *Let L satisfy the Legendre property. The Hamiltonian $H : \Omega \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ associated to L reads:*

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

We introduce two different definitions for the Hamiltonian functional $\mathcal{H}$: $\mathrm{Dom}(\mathcal{H}) \to \mathbb{R}$ associated to H with domain $\mathrm{Dom}(\mathcal{H}) \subset \mathrm{M} \times \mathrm{X}$:

1. *Primal Hamiltonian.*

$$\mathcal{H}(u,\mathbf{F}) := \int_\Omega \mathbf{F} \cdot \nabla u - H(x,u,\mathbf{F})\,dx. \tag{24}$$

2. *Dual Hamiltonian.*

$$\mathcal{H}(u,\mathbf{F}) := \int_\Omega -\operatorname{div}(\mathbf{F})u - H(x,u,\mathbf{F})\,dx. \tag{25}$$

For both the primal and the dual cases, we formally define $\mathrm{Dom}(\mathcal{H})$ as a subspace of $M \times X$ on which the Hamiltonian functional is well defined. For the primal case we have $\mathrm{Dom}(\mathcal{H}) \subset \mathrm{H}^1(\Omega) \times \mathrm{X}$ whereas for the dual case $\mathrm{Dom}(\mathcal{H}) \subset \mathrm{M} \times \mathrm{H}_{\mathrm{div}}(\Omega)$.

***Proposition 2*.** — *We consider a space of variations $V \times W \subset \mathrm{Dom}(\mathcal{H})$. Following the definitions in section 4, the Hamiltonian functional $\mathcal{H}$ is differentiable at point $(u,\mathbf{F}) \in \mathrm{Dom}(\mathcal{H})$ if*

$$\frac{\partial H}{\partial y}(x,u,\mathbf{F}) \in M \quad \text{and} \quad \frac{\partial H}{\partial p}(x,u,\mathbf{F}) \in X.$$

In such a case we have:

– *In the primal case:*

(26)

$$D\mathcal{H}(u,\mathbf{F}) \cdot (v,\mathbf{G}) = \int_\Omega \left[\mathbf{G} \cdot \left(\nabla u - \frac{\partial H}{\partial p}(x,u,\mathbf{F})\right) + \nabla v \cdot \mathbf{F} - v\frac{\partial H}{\partial y}(x,u,\mathbf{F})\right] dx.$$

– *In the dual case:*

$$D\mathcal{H}(u,\mathbf{F})\cdot(v,\mathbf{G}) = \int_\Omega \left[-\operatorname{div}(\mathbf{G})u - \mathbf{G}\cdot\frac{\partial H}{\partial p}(x,u,\mathbf{F}) - v\left(\operatorname{div}\mathbf{F} + \frac{\partial H}{\partial y}(x,u,\mathbf{F})\right)\right] dx.$$

***Definition 16* (Extremals).** — *Let us consider a space of variation* $V\times W \subset \operatorname{Dom}(\mathcal{H})$. *We say that* $(u,\mathbf{F})\in\operatorname{Dom}(\mathcal{H})$ *is an extremal for* $\mathcal{H}$ *relatively to* $V\times W$ *if* $\mathcal{H}$ *is differentiable at point* $(u,\mathbf{F})$ *and:*

$$D\mathcal{H}(\mathbf{F},u)\cdot(\mathbf{G},v) = 0 \quad \forall\ (v,\mathbf{G})\in V\times W.$$

***Theorem 6* (Hamilton's least action principle).** — *Let* $(u,\mathbf{F})\in\operatorname{Dom}(\mathcal{H})$ *be an extremal for* $\mathcal{H}$ *relatively to* $V\times W$. *Assume moreover that:*

- *in the primal case:* $\mathbf{F}\in H_{\mathrm{div}}(\Omega)$, $V_0=\{v\in V, v=0 \text{ on } \partial\Omega\}$ *is dense in* M *and* W *is dense in* X,
- *in the dual case:* $u\in H^1(\Omega)$, V *is dense in* M *and* $W_0=\{\mathbf{G}\in W, \mathbf{G}\cdot n = 0 \text{ on } \partial\Omega\}$ *is dense in* X.

Then $(u,\mathbf{F})$ *is a solution of the Hamiltonian system:*

$$\begin{cases} \operatorname{div}\mathbf{F} &= -\dfrac{\partial H}{\partial y}(x,u,\mathbf{F}) \\ \nabla u &= \dfrac{\partial H}{\partial p}(x,u,\mathbf{F}). \end{cases} \tag{27}$$

Proof. — Let us consider the case of the primal definition of the Hamiltonian functional $\mathcal{H}$. Since $\mathbf{F}\in H_{\mathrm{div}}(\Omega)$, using the Green formula in (26) gives: $\forall (v,\mathbf{G})\in V\times W$,

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

The boundary integral vanishes for $v\in V_0$. We recover (27) by density of V_0 in M and of W in X. ☐

***Corollary 1* (Lagrangian and Hamiltonian formulations)**

The solutions $(u,\mathbf{F})$ *of the Hamiltonian system* (27) *are exactly the solutions of the Euler-Lagrange equation* (5) *under the condition*

$$\mathbf{F} := \frac{\partial L}{\partial v}\big(x,u,\nabla_x u)\big).$$

9.2. Application to the Poisson problem. — We consider problem (7). We recall that the Lagrangian function associated with this problem is

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

The Legendre property is clearly satisfied by L since $\dfrac{\partial L}{\partial v}(x,y,v) = \alpha(x)v$. We introduce the new variable $p=\alpha(x)v$ and the function g is given by $g(x,y,p) = \alpha^{-1}(x)p$. A Hamiltonian for the Poisson equation is then given by

$$H(x,y,p) = p\cdot\big(\alpha^{-1}(x)p\big) - L(x,y,g(x,y,p)) = \frac{1}{2}\alpha^{-1}(x)p\cdot p + f(x)y. \tag{28}$$

Proposition 3. — *The Hamiltonian system* (27) *associated with* (28) *is the mixed formulation of the Poisson problem* (7)*:*

$$\begin{cases} -\operatorname{div}\mathbf{F} &= f \\ \nabla u &= \alpha^{-1}(x)\mathbf{F}\,. \end{cases} \tag{29}$$

The mixed problem (29) together with the homogeneous Dirichlet boundary condition $u = 0$ on $\partial\Omega$ has the classical mixed weak formulations:

1. Primal formulation: look for $(u, \mathbf{F}) \in H^1_0(\Omega) \times X$ such that

$$\begin{cases} -(\mathbf{F}, \nabla v)_{0,\Omega} = -(f, v)_{0,\Omega}\,, & \forall v \in H^1_0(\Omega) \\ (\alpha^{-1}\mathbf{F} - \nabla u, \mathbf{G})_{0,\Omega} = 0\,, & \forall \mathbf{G} \in X \end{cases} \tag{30}$$

2. Dual formulation: look for $(u, \mathbf{F}) \in M \times H_{\text{div}}(\Omega)$ such that

$$\begin{cases} (\operatorname{div}\mathbf{F} + f, v)_{0,\Omega} = 0\,, & \forall v \in M \\ (\alpha^{-1}\mathbf{F}, \mathbf{G})_{0,\Omega} + (u, \operatorname{div}\mathbf{G})_{0,\Omega} = 0\,, & \forall \mathbf{G} \in H_{\text{div}}(\Omega) \end{cases} \tag{31}$$

Proposition 4. — *A solution for* (30) *is an extremal* $(u, \mathbf{F}) \in H^1_0(\Omega) \times X$ *for the primal definition* (24) *of* $\mathcal{H}$ *relatively to the space of variations* $V \times W = H^1_0(\Omega) \times X$*.*

A solution for (31) *is an extremal* $(u, \mathbf{F}) \in M \times H_{\text{div}}(\Omega)$ *for the dual definition* (25) *of* $\mathcal{H}$ *relatively to the space of variations* $V \times W = M \times H_{\text{div}}(\Omega)$*.*

10. Discrete Hamiltonian and Coherence

Let us consider a discretised version of the mixed problem (27) obtained by some numerical scheme. If the discrete problem is also an extremal of a discrete Hamiltonian functional the considered numerical scheme is said to be coherent. It is the analogue of definition 8 to the Hamiltonian functional. Let us precise here the notion of coherence regarding Hamiltonian structures. We assume we have two discrete spaces M_h and X_h and an equation on $M_h \times X_h$ that we refer to as the *discrete differential embedding for PDE* (27). On the other hand assume that we have a discrete Hamiltonian $\mathcal{H}_h :\ M_h \times X_h \to \mathbb{R}$. If the solutions $(u_h, \mathbf{F}_h)$ of the discrete differential embedding for system of PDEs (27) are the solutions of the discrete least action principle $D\mathcal{H}_h(u_h, \mathbf{F}_h) = 0$ then the discretisation is said *coherent*. This can be summarised by saying that the following diagram commutes:

$$\begin{array}{ccc} (u,\mathbf{F}) \in M \times X \mapsto \mathcal{H}(u,\mathbf{F}) & \xrightarrow{\text{disc. var. emb.}} & (u_h,\mathbf{F}_h) \in M_h \times X_h \mapsto \mathcal{H}_h(u_h,\mathbf{F}_h) \\ \text{L.A.P.}\downarrow & & \downarrow\text{disc. L.A.P.} \\ (u,\mathbf{F}) \text{ solution of PDE (27)} & \xrightarrow{\text{disc. diff. emb.}} & (u_h,\mathbf{F}_h) \text{ solution of PDE}_h \\ \text{(Hamiltonian system)} & & \text{(discrete Hamiltonian system)} \end{array}$$

Remark 6 **(Coherence for conforming mixed finite element)**

We point out here that the mixed finite element schemes naturally are coherent. Consider some classical discretisation M_h *and* X_h *of* M *and* X *(for example* $M_h = P^0(\mathcal{T}_h)$ *and* $X_h = RT^0(\mathcal{T}_h)$ *the Raviart-Thomas elements of order 0, see e.g.* [**16**]*). A discrete differential embedding of* (27) *given by the conforming mixed finite element* *method relatively to a homogeneous Dirichlet boundary condition reads: look for* $(u_h, \mathbf{F}_h) \in M_h \times X_h$ *such that for any* $(v_h, \mathbf{G}_h) \in M_h \times X_h$,

$$\int_\Omega \left[-\operatorname{div}(\mathbf{G}_h) u_h - \mathbf{G}_h \cdot \frac{\partial H}{\partial p}(x, u_h, \mathbf{F}_h) - v_h \left(\operatorname{div} \mathbf{F}_h + \frac{\partial H}{\partial y}(x, u_h, \mathbf{F}_h) \right) \right] dx = 0.$$

A discrete variational embedding is provided by defining the discrete Hamiltonian $\mathcal{H}_h : M_h \times X_h \to \mathbb{R}$ *as the restriction of* $\mathcal{H}$ *to* $M_h \times X_h$. *This definition makes sense when considering conforming finite elements where* $X_h \subset H_{\mathrm{div}}(\Omega)$.
So defined, the discrete embeddings naturally are coherent.

Remark 7. — *Let us note that the definition of the Legendre property is not clear on the discrete level. As an example, considering again the Raviart-Thomas elements of order 0 for the mixed Poisson problem, we do not get* $\mathbf{F}_h = \nabla u_h$, *but some more complicated formula depending also on the source term* f.

11. Mimetic Finite Differences

We consider the mixed Poisson problem (29) together with a homogeneous Dirichlet condition $u = 0$ on $\partial\Omega$. The dual weak formulation (31) is adopted. The spaces of variations are set to $V = M = L^2(\Omega)$, and $W = X = H_{\mathrm{div}}(\Omega)$. The ambient space $M \times X$ is equipped with the following scalar products:

$$(u, v)_M = \int_\Omega uv \; dx \;, \quad (\mathbf{F}, \mathbf{G})_X = \int_\Omega \alpha^{-1} \mathbf{F} \cdot \mathbf{G} \; dx.$$

A flux operator $\mathcal{G} : H^1(\Omega) \subset M \longrightarrow X$ is introduced: $\mathcal{G}u = \alpha \nabla u$. This operator is adjoint to the divergence operator $\operatorname{div} : W \subset X \longrightarrow M$ in the following sense:

$$\forall \; u \in H^1_0(\Omega) \;, \quad \forall \; \mathbf{F} \in W \;\; : \quad (\mathbf{F}, \mathcal{G}u)_X = -\left(\operatorname{div} \mathbf{F}, u \right)_M \;.$$

In the Mimetic Finite Differences (MFD) framework, two discrete functional spaces M_h and W_h are introduced allowing to define discrete divergence $\operatorname{div}_h : W_h \longrightarrow M_h$. Scalars products on M_h and W_h are then introduced. A discrete flux operator is eventually introduces as (minus) the adjoint of the discrete divergence. We refer to [**4**] for the MFD discretisation of diffusion problems.

11.1. Discrete differential embedding. — A mesh $\mathcal{T}_h$ of the domain Ω is considered, the definitions and notations in definition 11 are adopted here. The discrete space M_h is set to be the space of piecewise constant functions on the mesh cells $K \in \mathcal{T}_h$ defined in (17). We consider the notations introduced in section 8 and the interpolation operator $I : u \in M \longrightarrow u^I \in M_h$ defined in (18) . We consider on M_h the scalar product induced by the Euclidean structure on M:

$$\forall u_h, v_h \in M_h : \; [u_h, v_h]_{M_h} = \sum_{K \in \mathcal{T}_h} u_K v_K |K|. \tag{32}$$

Fluxes are associated to each face $e \in \mathcal{E}$. To define such fluxes, a crossing direction has to be considered on the faces: to every cells $K \in \mathcal{T}_h$ and to every $e \in \mathcal{E}$ such that $e \subset \partial K$ we define $\mathbf{n}_{K,e}$ the unit normal to e pointing outward from K. Numerical fluxes $F_{K,e} \in \mathbb{R}$ are associated to each face e in the direction $\mathbf{n}_{K,e}$. We introduce the continuity condition:

$$\forall e = K_1 | K_2 \in \mathcal{E}_i : \; F_{K_1,e} + F_{K_2,e} = 0. \tag{33}$$

The discrete space W_h is defined as

$$W_h := \{(F_{K,e}) \text{ for } K \in \mathcal{T}_h,\ e \in \mathcal{E} \ \text{ s.t. } \ e \subset \partial K \text{ that satisfies (33)}\}\ .$$

The dimension of W_h is equal to the number $\#\mathcal{E}$ of faces in $\mathcal{E}$. However, no canonical isomorphism between W_h and $\mathbb{R}^{\#\mathcal{E}}$ is available: to define such an isomorphism necessitates to prescribe a crossing sense on each face $e \in \mathcal{E}$.
The following interpolation operator is considered:

$$\mathbf{F} \in W \mapsto \mathbf{F}^I \in W_h \ : \quad \mathbf{F}^I_{K,e} := \frac{1}{|e|}\int_e \mathbf{F}\cdot \mathbf{n}_{K,e} ds.$$

Definition 17. — *The discrete divergence* $\operatorname{div}_h :\ W_h \longrightarrow M_h$ *is defined as,*

$$\forall\ F_h \in W_h\ ,\quad \forall\ K \in \mathcal{T}_h\ ,\quad (\operatorname{div}_h F_h)_K := \frac{1}{|K|}\sum_{e\in\mathcal{E}, e\subset\partial K} F_{K,e}|e|.$$

For all $\mathbf{F} \in W$*, we have* $(\operatorname{div}\mathbf{F})^I = \operatorname{div}_h\left(\mathbf{F}^I\right)$*, meaning that the following diagram commutes:*

$$\begin{array}{ccc} W & \xrightarrow{\operatorname{div}} & M \\ {\scriptstyle I}\big\downarrow & & \big\downarrow{\scriptstyle I} \\ W_h & \xrightarrow{\operatorname{div}_h} & M_h \end{array}$$

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

$$\forall F_h, G_h \in W_h :\ [F_h, G_h]_{W_h} := \sum_{K\in\mathcal{T}_h}[F_h, G_h]_K, \tag{34}$$

the definition of $[\cdot,\cdot]_K$ will be detailed later on. Relatively to the scalar products (32) and (34), the discrete flux operator $\mathcal{G}_h : M_h \longrightarrow W_h$ is defined as (minus) the adjoint of the discrete divergence $\mathcal{G}_h = -\operatorname{div}_h^\star$, where $\star$ stands for the adjoint.

Problem (29) is then discretised as follows, [**4**]: find $u_h \in M_h$ and $F_h \in W_h$ such that,

$$\begin{cases} -\operatorname{div}_h F_h & = f^I \\ F_h - \mathcal{G}_h u_h & = 0 \end{cases}$$

which is equivalent with: find $u_h \in M_h$ and $F_h \in W_h$ such that,

$$\begin{cases} \forall\ v_h \in M_h, & [\operatorname{div}_h F_h, v_h]_{M_h} & = -[f^I, v_h]_{M_h} \\ \forall\ G_h \in W_h, & [F_h, G_h]_{W_h} + [u_h, \operatorname{div}_h G_h]_{M_h} & = 0 \end{cases}. \tag{35}$$

A way to define the elemental scalar product (34) is to introduce a lifting operator $\mathcal{R}_K : W_h^K \longrightarrow [L^2(K)]^d$ and then to define:

$$[F_h, G_h]_K := \int_K \alpha^{-1}(x)\mathcal{R}_K(F_h)\cdot\mathcal{R}_K(G_h)dx.$$

Consistency is ensured by imposing the three following conditions on the lifting operators. For all $K \in \mathcal{T}_h$ and all $F_h \in W_h^K$:

$$\forall\ e \in \mathcal{E},\ e \subset \partial K\ :\quad \mathcal{R}_K(F_h)\cdot\mathbf{n}_{K,e} = F_{K,e}\ ;\quad \operatorname{div}\left(\mathcal{R}_K(F_h)\right)) = \operatorname{div}_K\left(F_h\right);$$

and for all constant vector $\mathbf{c} \in \mathbb{R}^d$:

$$\mathcal{R}_K\left(\mathbf{c}^I\right) = \mathbf{c}.$$

11.2. Discrete variational embedding, coherence. — We consider the dual definition (25) for the Hamilton functional $\mathcal{H}$ on $M \times W$ relatively to H defined in (28). It reads:

$$\begin{aligned}\mathcal{H}(u, \mathbf{F}) &= \int_\Omega \alpha^{-1}\mathbf{F} \cdot \alpha\nabla u - \frac{1}{2}\int_\Omega \alpha^{-1}\mathbf{F}\cdot\mathbf{F} - \int_\Omega f(x)u \\ &= (\mathbf{F}, \mathcal{G}u)_X - \frac{1}{2}(\mathbf{F},\mathbf{F})_X - (u, f)_M .\end{aligned}$$

Definition 18 **(Discrete Hamiltonian)**. — *We therefore consider the following definition of the discrete Hamiltonian functional: $\mathcal{H}_h : M_h \times W_h \longrightarrow \mathbb{R}$:*

$$\mathcal{H}_h(u_h, F_h) := [F_h, \mathcal{G}_h u_h]_{W_h} - \frac{1}{2}[F_h, F_h]_{W_h} - \left[u_h, f^I\right]_{M_h} . \tag{36}$$

Theorem 7 **(Coherence)**. — *The MFD discretisation for the mixed Poisson problem (29) is coherent in the sense of section 10. Precisely: The discrete Hamiltonian $\mathcal{H}_h$ in (36) has a unique singular point $(u_h, F_h) \in M_h \times W_h$ such that*

$$D\mathcal{H}_h(u_h, F_h)(v_h, G_h) = 0 \quad \forall (v_h, G_h) \in M_h \times W_h.$$

This singular point is the unique solution to (35).

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

$$D\mathcal{H}_h(u_h, F_h)(v_h, G_h) = [F_h, \mathcal{G}_h v_h]_{W_h} + [\mathcal{G}_h u_h, G_h]_{W_h} - [F_h, G_h]_{W_h} - \left[f^I, v_h\right]_{M_h} .$$

A singular point (u_h, F_h) for $\mathcal{H}_h$ then satisfies:

$$\begin{cases} \forall\, v_h \in M_h, & [F_h, \mathcal{G}_h v_h]_{W_h} = [f^I, v_h]_{M_h} \\ \forall\, G_h \in W_h, & [F_h, G_h]_{W_h} - [\mathcal{G}_h u_h, G_h]_{W_h} = 0 \end{cases},$$

which exactly reads (35) by using $\mathcal{G}_h = -\operatorname{div}_h^\star$.
One can easily prove that (35) has a unique solution. □

Notations

- Ω open bounded domain $\Omega \subset \mathbb{R}^d$,
- $\partial\Omega$ domain boundary,
- M scalar function space on Ω, $M = L^2(\Omega)$,
- X vector function space on Ω, $X = L^2(\Omega)^d$,
- L Lagrangian function $L : \Omega \times \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$,
- $\mathcal{L}$ Lagrangian functional $\mathcal{L} : M \longrightarrow \mathbb{R}$,
- H Hamiltonian function $H : \Omega \times \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$,

- $\mathcal{H}$ Hamiltonian functional $\mathcal{H} : M \times X \longrightarrow \mathbb{R}$,
- $_h$ index for all discrete objects.
- $\mathcal{T}_h$ mesh of Ω,
- $\mathcal{E}$ mesh faces (or edges in dimension 2),
- $\mathcal{E}_0$ boundary faces,
- $\mathcal{E}_i$ internal faces,
- $\mathcal{N}$ vertices set,
- K one cell (or control volume) of $\mathcal{T}_h$,
- e one face (or edge) of $\mathcal{T}_h$,
- $|\cdot|$ object measure (according to its dimension),
- $H^m(\Omega)$ denotes the Sobolev space of order m,
- $\|v\|_{m,\Omega} = \left(\sum_{|\alpha|\leq m} \|\partial^\alpha v\|^2_{0,\Omega}\right)^{1/2}$,
- for any $f \in H^1(\Omega)$, its gradient is given by $\nabla f = \begin{pmatrix} \partial_{x_1} f \\ \partial_{x_2} f \\ \vdots \\ \partial_{x_d} f \end{pmatrix}$,

  we refer to $\nabla_x f$ to emphasise that the derivative is respect to the x parameter,
- the divergence of a vector F is $\operatorname{div} F = \sum_{i=1}^{d} \partial_{x_i} F_i$,
- $H^1_0(\Omega) = \left\{v \in H^1(\Omega),\ v_{|\partial\Omega} = 0\right\}$,
- $H_{\text{div}}(\Omega) = \{v \in (L^2(\Omega))^d,\ \operatorname{div} v \in L^2(\Omega)\}$.

References

[1] Vladimir I. Arnold. *Mathematical methods of classical mechanics*, volume 60 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, second edition, 1989. Translated from the Russian by K. Vogtmann and A. Weinstein.

[2] Loïc Bourdin, Jacky Cresson, Isabelle Greff and Pierre Inizan, Variational integrators on fractional Lagrangian systems in the framework of discrete embeddings, preprint, 2011.

[3] Franco Brezzi and Michel Fortin. Mixed and hybrid finite element methods. 15:x+350, 1991.

[4] Franco Brezzi, Konstantin Lipnikov, and Mikhail Shashkov. Convergence of the mimetic finite difference method for diffusion problems on polyhedral meshes. *SIAM J. Numer. Anal.*, 43(5):1872–1896 (electronic), 2005.

[5] Philippe G. Ciarlet. *The finite element method for elliptic problems*, volume 40 of *Classics in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2002. Reprint of the 1978 original [North-Holland, Amsterdam; MR0520174 (58 #25001)].

[6] Jacky Cresson, Fractional embedding of differential operators and Lagrangian systems, J. Math. Phys. **48** (2007), no. 3, 033504, 34 pp.

[7] Jacky Cresson, Introduction to embedding formalisms and PDEs, Lecture Notes TU München, 2011.

[8] Jacky Cresson and Sébastien Darses. Stochastic embedding of dynamical systems. *J. Math. Phys.*, 48(7):072703, 54, 2007.

[9] Jacky Cresson and Isabelle Greff. Non-differentiable embedding of Lagrangian systems and partial differential equations. *Preprint Max-Planck institute for the sciences, Leipzig,16/2010.*, page 19 p., 2010.

[10] Jacky Cresson, Isabelle Greff, and Pierre Inizan. A variational formulation for convection-diffusion problems. *Preprint*, 2011.

[11] Jacky Cresson and Pierre Inizan. Variational formulations of differential equations and asymmetric fractional embedding. *Journal of Mathematical Analysis and Applications (in revision)*, 2010.

[12] Lawrence C. Evans. *Partial differential equations*, volume 19 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, second edition, 2010.

[13] Robert Eymard, Thierry Gallouët, and Raphaèle Herbin. Finite volume methods. In *Handbook of numerical analysis, Vol. VII*, Handb. Numer. Anal., VII, pages 713–1020. North-Holland, Amsterdam, 2000.

[14] Mariano Giaquinta and Stefan Hildebrandt. *Calculus of variations. I*, volume 310 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, 1996. The Lagrangian formalism.

[15] Mariano Giaquinta and Stefan Hildebrandt. *Calculus of variations. II*, volume 311 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, 1996. The Hamiltonian formalism.

[16] Vivette Girault and Pierre-Arnaud Raviart. *Finite element methods for Navier-Stokes equations*, volume 5 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 1986. Theory and algorithms.

[17] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. Structure-preserving algorithms for ordinary differential equations.

[18] Jerrold E. Marsden and Matthew West. Discrete mechanics and variational integrators. *Acta Numer.*, 10:357–514, 2001.

[19] Vidar Thomée. Finite difference methods for linear parabolic equations. In *Handbook of numerical analysis, Vol. I*, Handb. Numer. Anal., I. North-Holland, Amsterdam, 1990.

June 20th, 2011

Jacky Cresson

Isabelle Greff

Charles Pierre