V European Conference on Computational Fluid Dynamics ECCOMAS CFD 2010 J. C. F. Pereira and A. Sequeira (Eds) Lisbon, Portugal,14-17 June 2010

# NUMERICAL SOLUTION OF ADVECTION EQUATIONS WITH THE DISCRETIZATION OF THE LIE DERIVATIVE

## A. Palha<sup>\*</sup>, J. Kreeft<sup>†</sup> and M. Gerritsma<sup>†</sup>

\*TUDelft, Faculty of Aerospace Engineering, Aerodynamics Group, Kluyverweg 2, 2629 HT Delft, The Netherlands e-mail: a.palha@tudelft.nl
<sup>†</sup>TUDelft, Faculty of Aerospace Engineering, Aerodynamics Group, Kluyverweg 2, 2629 HT Delft, The Netherlands e-mail: j.j.kreeft@tudelft.nl, m.i.gerritsma@tudelft.nl

**Key words:** Mimetic Discretization, Compatible Discretization, advection, Lie Derivative, Hodge-star

Abstract. It is well known that, for example, the application of the classical Galerkin finite element method is inappropriate for the solution of advection equations, at high Peclet numbers. Typically, unwanted spurious (non-physical) oscillations appear in the numerical solution. In the last three decades, several alternative schemes have been developed in order to reduce these unwanted artifacts. The authors consider that the unstable character of the numerical solutions lies in the inadequate discretization of the equations. That is, a discretization scheme that adequately mimics, in the sense that is preserves the same properties such as symmetries, conserved quantities, etc., of the continuous differential equations should, intrinsically, result in a stable scheme. Hence, in this work, a new approach is followed. Taking as basis the framework of differential geometry the authors present a mimetic discretization scheme for the advection equation which is mass and energy preserving.

### **1 INTRODUCTION**

Numerical schemes are an essential tool for solving PDE's. These schemes, being a model reduction, inherently lead to loss of information of the system being modeled, namely on its structure, e.g. conservation of certain quantities – mass, momentum, energy, etc. – and symmetries, which are embedded into the PDE's as a result of the geometrical properties of the differential operators. It is known today<sup>2,3,15,21</sup> that the well-posedness of many PDE problems reflects geometrical, algebraic topological and homological structures underlying the problem. It is, therefore, important for the numerical scheme to be compatible with these structures (the physics), i.e., to mimic them. The goal of mimetic methods is to satisfy exactly, or as good as possible, the structural properties of the continuous model, in doing so, one obtains stable schemes. Additionally, a clear separation between the processes of discretization and approximation arises, the latter only take place in the constitutive relations.

It is well known<sup>22</sup> that the application of the classical Galerkin finite element method, for high Peclet numbers, is inappropriate for the solution of advection equations with no source terms:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\boldsymbol{v}\rho) = 0 \quad (\boldsymbol{x}, t) \in \Omega \times [0, T], \quad \rho(t, \partial \Omega_{\rm in}) = \rho_b(t), \quad \rho(0, \boldsymbol{x}) = \rho_0(\boldsymbol{x}), \quad (1)$$

where  $\rho$  is the advected quantity and  $\boldsymbol{v}$  is the vector field that advects the quantity  $\rho$ . Typically, unwanted spurious (non-physical) oscillations appear in the numerical solution. In the last three decades, several alternative schemes have been developed<sup>22</sup> in order to attenuate these unwanted artifacts. The authors consider that the unstable character of the numerical solutions lies in the inadequate discretization of the equations. As said before, a discretization scheme that adequately mimics, that is, preserves the same properties such as symmetries, conserved quantities etc., of the continuous differential equations should, intrinsically, result in a stable scheme. Hence, in this work, a new approach is followed. It is known from differential geometry<sup>1,6</sup> that (1) is a specific case of a larger family of boundary value problems modeling convective phenomena. For a scalar advected quantity it is possible to express it in terms of the Hodge-\* operator, \*, and the Lie derivative,  $\mathcal{L}_{\beta}$ , in the following way:

$$\mathcal{L}_{\boldsymbol{\beta}} \star \boldsymbol{\omega}^0 = 0 \quad \text{in } \boldsymbol{\Omega} \in \mathbb{R}^m \tag{2}$$

This is then an equation that models the space-time advection of 0-forms. Discrete differential forms have shown to be a good approach for discretizing terms of the form  $\delta d\omega^k$ and  $d\delta\omega^k$ , and its implementations can be found in the literature<sup>2,3,5,9,15,17</sup>. Hence, the aim of this work is to take these ideas a step further and apply them to the discretization of the Lie derivative operator. Taking as a starting point previous work from other authors<sup>4,16</sup>, for the discretization of advection-like equations, the authors present a mimetic quadrilateral high order, spectral finite element method which, under some conditions, exactly conserves both the advected property and the energy associated with it. The path the authors will follow starts with an introduction to differential geometry, where a brief introduction to fundamental concepts such as vector fields, differential forms, exterior derivative, Hodge-\* operator and Lie derivative is given. Following this, discrete analogs of these concepts are presented. To finalize, these ideas are combined and applied to the advection problem and numerical results showing some of the properties of the derived scheme are presented.

## 2 DIFFERENTIAL GEOMETRY: A REFRESHER

The introduction presented here is done for a 2-dimensional manifold, since this will be dimension of the space to which the advection equation will be applied to, the generalization to higher dimensional manifolds is straightforward, all equations expressed using Einstein's notation are automatically extended to higher dimensions.

### 2.1 Vector fields

On a manifold,  $\mathcal{M}$ , the *tangent space* at a point, P, is usually thought of as a tangent plane to a surface. Although this is not incorrect it proves to be better to realize a tangent vector,  $\vec{v}$ , to be understood as something that is tangent to a *curve* that lies in the manifold. The important point here is that the curve lies exclusively in the manifold  $\mathcal{M}$ . The problem then, lies in the fact that different curves passing by the same point, P, are "tangent" to the vector  $\vec{v}$ . This leads to the idea of tangent vectors as equivalence classes of curves. A geometrical definition of tangent vector as an equivalence class of curves is<sup>13</sup>:

## Definition 1.

1. A curve on a manifold  $\mathcal{M}$  is a smooth (i.e.,  $C^{\infty}$ ) map  $\gamma$  from some interval  $(-\epsilon, \epsilon)$  of the real line into  $\mathcal{M}$ .

Note that the 'curve' is defined to be the map itself, not the set of image points in  $\mathcal{M}$ . It is important to remember this distinction between a function and its set of image points.

- 2. Two curves  $\gamma_1$  and  $\gamma_2$  are tangent at a point P in  $\mathcal{M}$  if
  - a)  $\gamma_1(0) = \gamma_2(0) = P;$
  - b) in some local coordinate system  $(x^1, x^2, ..., x^n)$  around the point, P, the two curves are 'tangent' in the usual sense as curves in  $\mathbb{R}^n$ :

$$\frac{dx^{i}}{dt}\left(\gamma_{1}(t)\right)\Big|_{t=0} = \frac{dx^{i}}{dt}\left(\gamma_{2}(t)\right)\Big|_{t=0}$$

for i = 1, 2, ..., n.

Note that if  $\gamma_1$  and  $\gamma_2$  are tangent in one coordinate system, then they are tangent in any other coordinate system that covers the point  $P \in \mathcal{M}$ . Thus the definition is an intrinsic one, i.e., it is independent of coordinate system.

- c) A tangent vector,  $\vec{v}$ , at  $P \in \mathcal{M}$  is an equivalence class of curves in  $\mathcal{M}$  where the equivalence relation between two curves is that they are tangent at the point P. The equivalence class of a particular curve  $\gamma$  will be denoted by  $[\gamma]$ . One says that  $\vec{v} = [\gamma]$ .
- d) The tangent space denoted by  $T_P \mathcal{M}$  to  $\mathcal{M}$  at a point  $P \in \mathcal{M}$  is the set of all tangent vectors at the point P.

The tangent bundle  $T\mathcal{M}$  is defined as  $T\mathcal{M} := \bigcup_{P \in \mathcal{M}} T_P \mathcal{M}$ .

It is possible to show<sup>13</sup> that the tangent space, defined in this way, is, in fact, a linear vector space with properly defined addition and multiplication by scalars.

Another, more algebraic, approach to tangent vectors is to define them as a derivation operator<sup>10</sup>:

### Definition 2.

A derivation,  $\underline{v}$ , at a point  $P \in \mathcal{M}$  is an operator acting on smooth real valued functions on  $\mathcal{M}$ , that is:

$$\underline{v}: C^{\infty}(\mathcal{M}) \to \mathbb{R}$$

satisfying:

(i) 
$$\underline{v}(af + bg) = a \underline{v}(f)|_P + b \underline{v}(g)|_P$$
,  $a, b \ constant$   
(ii)  $\underline{v}(f \cdot g) = g(P) \cdot \underline{v}(f)|_P + f(P) \cdot \underline{v}(g)|_P$ .

where  $f, g \in C^{\infty}(\mathcal{M})$ .

Using this definition it is possible to verify that  $\underline{v}(c) = 0$  for c a constant. This property, present in *derivation* operators is produced essentially due to crucial *Leibniz rule* in (ii), which is clearly analogous to the rule in elementary calculus for taking the derivative at a fixed point of the product of two functions. The space  $D_P\mathcal{M}$ , can now be introduced as:

#### Definition 3.

The set of all derivations at  $P \in \mathcal{M}$  is denoted by  $D_P \mathcal{M}$ .

It is possible to endow this set with the structure of a vector space, by defining addition and multiplications by scalars in the following way:

$$(\underline{v}_1 + \underline{v}_2)(f) := \underline{v}_1(f) + \underline{v}_2(f)$$
  

$$(\underline{k}\underline{v})(f) := \underline{k}\underline{v}(f)$$
(3)

for all  $\underline{v}_1, \underline{v}_2, \underline{v} \in D_P \mathcal{M}, f \in C^{\infty}$  and  $k \in \mathbb{R}$ .

Now, it is possible to show<sup>10,13</sup> that in a local coordinate system,  $(\xi^1, \xi^2, \ldots, \xi^n)$ , valid in some neighborhood of P the following set of operators are a basis for the linear space  $D_P \mathcal{M}$ :

$$\partial_i = \left. \frac{\partial}{\partial \xi^i} \right|_P$$

The proof involves the linear approximation of a function f, using a Taylor expansion, and then the application of  $\underline{v} \in D_P \mathcal{M}$  to the linear approximation, using the above shown property that  $\underline{c} = 0$ . Hence, for any element  $D_P \mathcal{M}$ :

If 
$$\underline{v} \in D_P \mathcal{M} \Rightarrow \underline{v} = v^i \partial_i$$

where Einstein's notation was used, in order to imply summation over i.

The connection between the objects of  $D_P \mathcal{M}$  and the ones of  $T_P \mathcal{M}$  is made in the following way. First recall that the directional derivative of a function f along a vector  $\vec{v} \in T_P \mathcal{M}$  is defined as:

$$\vec{v}(f) := \left. \frac{d \left[ f \circ \gamma \right](t)}{dt} \right|_{t=0} \quad \text{where } \left[ \gamma \right] = \vec{v} \in T_P \mathcal{M}$$

which enables the equivalence class of curves,  $\vec{v} \in T_P \mathcal{M}$  to act as a differential operator on the space  $C^{\infty}(\mathcal{M})$  of real valued differentiable functions on  $\mathcal{M}$ . Expanding the right hand side yields:

$$\vec{v}(f)|_P := \left. \frac{d\gamma^i(t)}{dt} \frac{\partial f}{\partial \xi^i} \right|_{t=0} = \left( \frac{d\gamma^i(t)}{dt} \frac{\partial}{\partial \xi^i} \right) f \Big|_{t=0}$$

Looking at the last equality it is easy to identify that:

$$\left. \frac{d\gamma^i(t)}{dt} \right|_{t=0} \frac{\partial}{\partial \xi^i} \in D_P \mathcal{M}$$

Hence it is straight forward to introduce the linear map  $\sigma : T_P \mathcal{M} \to D_P \mathcal{M}$  defined in the following way:

$$\sigma(\vec{v}) := \left. \frac{d\gamma^i(t)}{dt} \right|_{t=0} \frac{\partial}{\partial \xi^i} = \underline{v}, \quad \text{where } [\gamma] = \vec{v}$$

It is possible to show<sup>13</sup> that, in fact, this mapping,  $\sigma$ , is an isomorphism and hence one can use one or the other space whenever it suits better.

Given the definitions of tangent vector and tangent space, the introduction of the concept of vector field is straightforward  $^{12,13,19}$ :

### Definition 4.

Let  $\mathcal{M}$  be a  $C^{\infty}$  manifold. A vector field X on  $\mathcal{M}$  is an assignment, to each point  $P \in \mathcal{M}$ , of a tangent vector  $X_P \in T_P \mathcal{M}$ , in such a way that  $X_P$  is smooth, that is, it is of class  $C^{\infty}$  with respect to P: for all  $f \in C^{\infty}(\mathcal{M})$ , the function  $Xf : \mathcal{M} \to \mathbb{R}$  defined by:

$$\mathcal{M} \to \mathbb{R}$$
  
 $P \mapsto [X(f)](P) := X_P(f)$ 

X is a section of the tangent bundle  $T\mathcal{M}$ .

In a local coordinate system of  $\mathcal{M}$ , for each point  $P \in \mathcal{M}$ , X is described as:  $X_P = a^i(P) \partial_i$ , where the  $a^i$  are functions defined in the local coordinates,  $(\xi^1, \ldots, \xi^n)$ . Note, however, that the local coordinates are not unique and hence, the geometrical properties of the vector field do not depend on them. Let  $(y^1, \ldots, y^n)$  be another local coordinate system, then:

$$X_p = \sum_{i,j} a^i(P) \frac{\partial y_j}{\partial x_i} \frac{\partial}{\partial y_j}$$

This transformation of coordinate system does not change the geometrical object. It is possible to endow a vector space with additional structure, namely an inner product. In Euclidean space the trivial inner product of two vectors  $\underline{a} = a^i \partial_i$  and  $\underline{b} = b^i \partial_i$  is simply given by:

$$(\underline{a},\underline{b}) = \sum_{i} a^{i} b^{i} = a^{i} b^{k} \delta_{ki}$$

$$\tag{4}$$

This implies implicitly that  $(\partial_i, \partial_j) = \delta_{ij}$ . This is not true, in general. Hence a metric, g, is introduced<sup>19</sup>:

## Definition 5.

Let  $\mathcal{M}$  be a manifold, if for each point  $P \in \mathcal{M}$  the tangent space  $T_P\mathcal{M}$  is provided with a positive-definite inner product,  $g_P(\cdot, \cdot)$  or  $(\cdot, \cdot)_P$ :

$$g_P: T_P\mathcal{M} \times T_P\mathcal{M} \to \mathbb{R}$$

in such a way that  $g_P$  is of class  $C^{\infty}$  in P, we say that  $g = \{g_P; P \in \mathcal{M}\}$  is a Riemannian metric on  $\mathcal{M}$ . One also says that  $\mathcal{M}$  equipped with g is a Riemannian manifold.

It is straightforward to see that, for a given coordinate system a metric is defined by a tensor with the following entries:

$$g_{ij} = (\partial_i, \partial_j) \tag{5}$$

In this way the inner product between two tangent vectors of a Riemannian manifold,  $\underline{a} = a^i \partial_i$  and  $\underline{b} = b^i \partial_i$ , becomes:

$$(\underline{a},\underline{b}) = a^i b^j g_{ij}$$

Hence, the introduction of the delta kronecker,  $\delta_{ki}$ , in (4), in Euclidean space:  $g_{ij} := (\partial_i, \partial_j) = \delta_{ij}$ .

One way of assigning a metric is through the use of an embedding. The inner product between two vectors in  $\mathcal{M}$  is then given by the Euclidean inner product in the higher dimensional Euclidean space where the embedding takes place.

#### 2.2 Differential forms

Having defined a tangent vector and the tangent space, one can introduce differential 1-forms, that is *cotangent vectors*, and the *cotangent space*:

#### Definition 6.

A cotangent vector,  $\omega$ , at a point  $P \in \mathcal{M}$  is a mapping of  $T_P \mathcal{M}$  to the real line:

 $\omega: T_P \mathcal{M} \to \mathbb{R}$ 

that satisfies the following property:

$$\omega(a\underline{v} + b\underline{w}) = a\omega(\underline{v}) + b\omega(\underline{w})$$

The set of all cotangent vectors at a point  $P \in \mathcal{M}$  is called the cotangent space,  $T_P^*\mathcal{M}$ . The set of all cotangent spaces is denoted by cotangent bundle:

$$T^*\mathcal{M} := \bigcup_{p\in\mathcal{M}} T^*_P\mathcal{M}.$$

If  $T_P^*\mathcal{M}$  is equipped with the following definitions for the addition of elements and multiplication by scalars, one obtains a linear vector space:

$$[\alpha + \beta](\underline{v}) = \alpha(\underline{v}) + \beta(\underline{v})$$
$$[k\alpha](\underline{v}) = k(\alpha(\underline{v}))$$

with  $\alpha, \beta \in T_P^*\mathcal{M}, \ \underline{v} \in T_P\mathcal{M}$  and  $k \in \mathbb{R}$ . Having in mind the Riesz representation theorem<sup>7</sup>, one has that:

$$\forall \omega \in T_P^* \mathcal{M} \; \exists \underline{w} \in T_P \mathcal{M} \; \mid \; \forall \underline{v} \in T_P \mathcal{M} \; \omega(\underline{v}) = (\underline{w}, \underline{v})$$

and one says that  $\omega$  is the dual of  $\underline{w}$ , and writes:  $\omega = \underline{w}^*$ . In this way one also refers to  $T_P^*\mathcal{M}$  (or in some contexts  $\Lambda^1$ ) as the dual space of  $T_P\mathcal{M}$ . Where  $(\underline{w}, \underline{v})$  is the *inner* product of  $\underline{w}$  and  $\underline{v}$ , see subsection 2.1.

One can go a step further and try to find a set of basis elements for this dual space, in the same way it was done for the tangent space. By definition, there is an infinite number of sets of basis elements, one is free to choose any one of them. A typical and easy choice is to choose a specific set, denoted by  $d\xi^i$ , such that:

$$d\xi^i(\partial_j) = \delta^i_j \tag{6}$$

It is important to note that this relation does not imply that in no way  $d\xi^i$  it the dual of  $\partial_i$ , it only specifies the action of the elements of the basis of  $T_P^*\mathcal{M}$  on the elements of  $T_P\mathcal{M}$ . To see how the duality pairing is one needs to use the Riesz representation theorem. This states that if  $\partial_i^* \in T_P^*\mathcal{M}$  is the dual of  $\partial_i \in T_P\mathcal{M}$  then:

$$\partial_i^*(\partial_j) = (\partial_i, \partial_j) \tag{7}$$

But also, since  $\partial_i^* \in T_P^* \mathcal{M}$  it must be represented as a linear combination of the basis elements:

$$\partial_i^* = c_{ik} d\xi^k \tag{8}$$

But putting (7) and (8) together, yields:

$$c_{ik}d\xi^k(\partial_j) = (\partial_i, \partial_j) \tag{9}$$

using (6) and (5) one sees that:

$$c_{ik}\delta_j^k = c_{ij} = (\partial_i, \partial_j) = g_{ij} \tag{10}$$

With this equation it is straightforward to introduce the so called musical isomorphisms: the flat operator,  $\flat$ , and the sharp operator,  $\sharp$ .

#### Definition 7.

The  $\flat$  operator,  $\flat : T_P \mathcal{M} \mapsto T_P^* \mathcal{M}$ , is an operator that maps the elements of the  $T_P \mathcal{M}$  into their dual elements in  $T_P^* \mathcal{M}$  in the following way:

$$\flat: \partial_i \longmapsto \partial_i^* = g_{ij} d\xi^j$$

where  $g_{ij} = (\partial_i, \partial_j)$ .

Due to this relation, it is possible to transform tangent vectors into cotangent vectors in the following way:

$$\flat : \underline{w} = w^i \partial_i \longmapsto \underline{w}^* = \underline{w}^\flat = w^i g_{ij} d\xi^j, \quad \forall \underline{w} \in T_P \mathcal{M}$$
(11)

If one looks at this operation in matrix form, one sees that one set of coefficients is transformed into the other simply multiplying by a matrix whose coefficients are the  $g_{ij}$  coefficients introduced in (10):

$\left[ \omega^1 \right]$		$\int g_{11}$	•••	$g_{1n}$ -	$\begin{bmatrix} w^1 \end{bmatrix}$
	=	÷	۰.	÷	
$\omega^n$		$g_{n1}$	•••	$g_{nn}$	$\begin{bmatrix} w^n \end{bmatrix}$

hence, inverting the matrix, one gets the inverse transformation:

#### **Definition 8.**

The  $\sharp$  operator,  $\sharp : T_P^* \mathcal{M} \mapsto T_P \mathcal{M}$ , is an operator that maps the elements of the  $T_P^* \mathcal{M}$  into their dual elements in the  $T_P \mathcal{M}$  in the following way:

$$\sharp: d\xi^i \longmapsto \left(d\xi^i\right)^* = \left(d\xi^i\right)^\sharp = g^{ij}\partial_j$$

Where the coefficients  $g^{ij}$  are the coefficients of the inverse matrix of the matrix whose coefficients are the metric coefficients,  $g_{ij}$ , and hence:  $g^{ik}g_{nk} = g^{ik}g_{kn} = \delta_n^i$ , where for the first equality the fact that the metric is symmetric was used to interchange indices.

For the cotangent space,  $T_P^*\mathcal{M}$ , given the inner product defined for the tangent space,  $T_P\mathcal{M}$ , in subsection 2.1, one can induce an inner product in the following way:

#### Definition 9.

Let  $\mathcal{M}$  be a manifold, each point  $P \in \mathcal{M}$  of the cotangent space  $T_P^*\mathcal{M}$  can be provided with a positive-definite inner product,  $g_P(\cdot, \cdot)$  or  $(\cdot, \cdot)_P$ :

$$g_P: T_P^*\mathcal{M} \times T_P^*\mathcal{M} \to \mathbb{R}$$

given by, for  $\alpha, \beta \in T_P^* \mathcal{M}$ :

$$(\alpha,\beta) := (\alpha^{\sharp},\beta^{\sharp})$$

Where  $(\alpha^{\sharp}, \beta^{\sharp})$  is the inner product of the tangent vectors  $\alpha^{\sharp}$  and  $\beta^{\sharp}$ , duals of  $\alpha$  and  $\beta$ , respectively, and the definition (5), of inner product of tangent vectors, and the definition (8), of sharp operator, were used.

In this way, and in local coordinates, the inner product between two cotangent vectors of a Riemannian manifold,  $\alpha = \alpha_i d\xi^i$  and  $\beta = \beta_i d\xi^i$ , becomes:

$$(\alpha,\beta) = \alpha_i \beta_j g^{ij}$$

Coordinate representations are different but they render coordinate free geometrical properties such as angles and lengths.

#### 2.3 Wedge product and k-forms

It was seen previously in Section 2.2, that any 1-form,  $\alpha^1$ , can be written, in a particular coordinate system, using the basis 1-forms  $d\xi^i$ , as:

$$\alpha^1 = \alpha_i d\xi^i \tag{12}$$

It was also seen in definition (6) that differential forms,  $\alpha^1 = \alpha_i d\xi^i \in T_P^* \mathcal{M}$ , are functionals,  $\omega : T_P \mathcal{M} \to \mathbb{R}$ , acting on tangent vectors  $\underline{v} = v^i \partial_i \in T_P \mathcal{M}$  such that:

$$\alpha^1(\underline{v}) = \alpha_i v^i \tag{13}$$

independent of the coordinate system, due to the transformation of vectors and 1-forms.

Several operators acting on differential forms will be introduced here. The most simple one being the *tensor product*,  $\otimes$ , of *m* 1-forms,  $_i\alpha^1 \in T_P^*\mathcal{M}$ :

$${}_{1}\alpha^{1}\otimes\cdots\otimes{}_{i}\alpha^{1}\otimes\cdots\otimes{}_{m}\alpha^{1}:T_{P}\mathcal{M}\times\cdots\times T_{P}\mathcal{M}\times\cdots T_{P}\mathcal{M}\mapsto\mathbb{R}$$
(14)

which, for  $\underline{v} \in T_P \mathcal{M}$ , is defined in the following way:

$${}_{1}\alpha^{1}\otimes\cdots\otimes{}_{i}\alpha^{1}\otimes\cdots\otimes{}_{m}\alpha^{1}({}_{1}\underline{v},\cdots,{}_{i}\underline{v},\cdots,{}_{m}\underline{v}) := {}_{1}\alpha^{1}({}_{1}\underline{v})\cdots{}_{i}\alpha^{1}({}_{i}\underline{v})\cdots{}_{m}\alpha^{1}({}_{m}\underline{v})$$
(15)

A particularly important combination of tensor products is the wedge product,  $\wedge$ :

$$\wedge: T_P^*\mathcal{M} \times T_P^*\mathcal{M} \mapsto T_P^*\mathcal{M} \otimes T_P^*\mathcal{M}$$
(16)

which, for  $\alpha^1, \beta^1 \in T^*_P \mathcal{M}$ , is defined in the following way:

$$\alpha^1 \wedge \beta^1 := \alpha^1 \otimes \beta^1 - \beta^1 \otimes \alpha^1 = \sigma^2 \tag{17}$$

Where  $\sigma^2 \in T_P^* \mathcal{M} \times T_P^* \mathcal{M}$  is an anti-symmetric differential form of rank 2, a 2-form. The space of all anti-symmetric 2-forms is denoted by  $\Lambda^2$ . Using (17) it is easy to show that the wedge product has the following properties:

$$\alpha^1 \wedge \beta^1 = -\beta^1 \wedge \alpha^1 \quad \text{and} \quad \alpha^1 \wedge \alpha^1 = 0$$
 (18)

It is possible<sup>20</sup> to construct higher rank forms, k-forms, by wedging and adding k 1-forms. The way to compute the wedge product between more than two 1-forms is shown for the case of  $\alpha^1 \wedge \beta^1 \wedge \gamma^1$ :

$$\begin{aligned} \alpha^{1} \wedge \beta^{1} \wedge \gamma^{1} &= (\alpha^{1} \otimes \beta^{1} - \beta^{1} \otimes \alpha^{1}) \wedge \gamma^{1} \\ &= (\alpha^{1} \otimes \beta^{1} - \beta^{1} \otimes \alpha^{1}) \otimes \gamma^{1} - \gamma^{1} \otimes (\alpha^{1} \otimes \beta^{1} - \beta^{1} \otimes \alpha^{1}) \\ &= \alpha^{1} \otimes \beta^{1} \otimes \gamma^{1} - \beta^{1} \otimes \alpha^{1} \otimes \gamma^{1} - \gamma^{1} \otimes \alpha^{1} \otimes \beta^{1} + \gamma^{1} \otimes \beta^{1} \otimes \alpha^{1} \\ &= \sigma^{3} \end{aligned}$$
(19)

Where  $\sigma^3 \in T_P^*\mathcal{M} \times T_P^*\mathcal{M}$  is a completely anti-symmetric differential form of rank 3, a 3-form. Analogously, the space of all anti-symmetric 3-forms is designated by  $\Lambda^3$ . This process is easily extended to higher ranks, hence it is adequate to refer to  $\Lambda^k$  as the space of all anti-symmetric k-forms, and  $\Lambda^0$  is the space of scalar functions, by definition. In a coordinate basis a 1-form can be written as  $\alpha^1 = \alpha_i d\xi^i$  hence, following the definition of wedge product any k-form,  $\sigma^k \in \Lambda^k$  can be written as:

$$\sigma^k = \sigma_{i_1 \dots i_k} d\xi^{i_1} \wedge \dots \wedge d\xi^{i_k}, \quad i_i < \dots < i_k \tag{20}$$

note that Einstein's notation is used, implying summation over repeated indices.

Having in mind that in a manifold  $\mathcal{M}$  of dimension n, there are only n linearly independent basis 1-forms, one can show that, at most, in a manifold of dimension n there are differential forms of maximum rank n, that is, n-forms. Hence, in this way one can state that the wedge product is an operator:

$$\wedge : \Lambda^k \times \Lambda^l \mapsto \Lambda^{k+l}, \qquad k+l < n, \tag{21}$$

And, by definition:

$$\alpha^0 \wedge \beta^1 := \alpha^0 \beta^1, \quad \forall \alpha^0 \in \Lambda^0, \, \forall \beta^1 \in \Lambda^1$$
(22)

### 2.4 Exterior derivative

The *exterior derivative*, d, plays an important role in differential geometry and in a n-dimensional space, is a mapping:

$$d: \Lambda^k \mapsto \Lambda^{k+1}, \qquad k = 0, 1, \dots, n-1,$$
(23)

which satisfies:

$$d\left(\omega^k \wedge \alpha^l\right) = d\omega^k \wedge \alpha^l + (-1)^k \omega^k \wedge d\alpha^l, \qquad k+l < n$$
(24)

and

$$dd\alpha^k := 0, \quad \forall \alpha^k \in \Lambda^k \tag{25}$$

and is defined for 0-forms,  $\alpha^0 \in \Lambda^0$ , as:

$$d\alpha^0 := \frac{\partial \alpha^0}{\partial \xi^i} d\xi^i \tag{26}$$

Having in mind (22),  $\alpha^1 = \alpha_i d\xi^i := \alpha_i \wedge d\xi_i$ , and using (24):

$$d\alpha^{1} := d(\alpha_{i} \wedge d\xi_{i}) := (d\alpha_{i}) \wedge d\xi^{1} + \alpha^{0} \wedge dd\xi^{i} = (d\alpha_{i}) \wedge d\xi^{1}$$

$$(27)$$

Where (25) was used. This equation can be further expanded into:

$$d\alpha^1 = \frac{\partial \alpha_i}{\partial \xi^j} d\xi^j \wedge d\xi^i \tag{28}$$

It follows directly that, on an *n*-dimensional manifold:

$$d\alpha^n = 0, \quad \forall \alpha^n \in \Lambda^n \tag{29}$$

It is possible to show<sup>6</sup> that differential k-forms are naturally integrated over k-dimensional manifolds. Moreover it is also possible to prove *Stokes' theorem* which generalizes several integral theorems of vector calculus:

$$\int_{\Omega^{k+1}} d\alpha^k = \int_{\partial\Omega^{k+1}} \alpha^k \tag{30}$$

## 2.5 Hodge- $\star$

The Hodge- $\star$  operator,  $\star$ , on an n-dimensional manifold, is a mapping:

$$\star : \Lambda^k \mapsto \Lambda^{n-k}, \qquad k \le n, \tag{31}$$

that satisfies:

$$\alpha \wedge \star \beta = (\alpha, \beta) \,\omega^n, \qquad \forall \alpha, \beta \in \Lambda^k. \tag{32}$$

where  $\omega^n$  is the normalized volume form defined as  $\omega^n := 1 \wedge \star 1$  and given on a coordinate system as  $\omega^n = \sqrt{|g|} d\xi^1 \wedge \ldots \wedge d\xi^n$ . One important point to note here is the fact that, contrary to the exterior derivative, d, the Hodge- $\star$  is metric dependent and hence local in nature, since the metric has a local nature. As will be seen in Section 3, metric dependent operators turn out to be the most difficult to discretize and are the ones where all approximation takes place. Hence, one can say that the crucial point of a proper discretization lies in the discretization of the Hodge- $\star$  and of the interior product,  $\iota_{\underline{v}}$ , with a vector field,  $\underline{v}$ . It is also important to introduce the  $L^2$  inner product of two k-forms,  $\alpha^k, \beta^k \in \Lambda^k, \langle \alpha^k, \beta^k \rangle$ :

$$\langle \alpha^k, \beta^k \rangle := \left( \alpha^k, \beta^k \right) \omega^n \tag{33}$$

where  $\omega^n$  is the normalized volume form defined previously.

## 2.6 Interior product and Lie derivative

The *interior product*,  $\iota_{\underline{v}}$ , of a vector  $\underline{v}$ , acting a differential k-form,  $\alpha^k$ , is a linear mapping:

$$\iota_{\underline{v}} \colon \Lambda^k \mapsto \Lambda^{k-1} \tag{34}$$

Defined in the following way on 1-forms,  $\alpha^1 \in \Lambda^1$ :

$$\iota_{\underline{v}}\alpha^1 := \alpha^1(\underline{v}), \quad \forall \alpha^1 \in \Lambda^1, \quad \underline{v} \in T_P \mathcal{M}$$
(35)

and in the following way on 0-forms:

$$\iota_{\underline{v}}\alpha^0 := 0, \quad \forall \alpha^0 \in \Lambda^0, \quad \underline{v} \in T_P \mathcal{M}$$
(36)

and with the following distribution property with the wedge product,  $\wedge$ :

$$\iota_{\underline{v}}(\alpha^p \wedge \beta^q) := (\iota_{\underline{v}}\alpha^p) \wedge \beta^q) + (-1)^p \alpha^p \wedge (\iota_{\underline{v}}\beta^q), \quad \forall \alpha^p \in \Lambda^p, \beta^q \in \Lambda^q, \quad \underline{v} \in T_P \mathcal{M}$$
(37)

The Lie derivative,  $\mathcal{L}_{\underline{v}}$ , acting a differential k-form,  $\alpha^k$ , is a linear mapping:

$$\mathcal{L}_{\underline{v}}: \Lambda^k \mapsto \Lambda^k \tag{38}$$

Using Cartan's magic formula one can express the Lie derivative,  $\mathcal{L}_{\underline{v}}$  as:

$$\mathcal{L}_{\underline{v}} := d\iota_{\underline{v}} + \iota_{\underline{v}}d \tag{39}$$

Given the properties of the interior product,  $\iota_{\underline{v}}$ , and of the exterior derivative, d, it follows directly that, on an *n*-dimensional manifold:

$$\mathcal{L}_{\underline{v}}\alpha^{0} = \iota_{\underline{v}}d\alpha^{0}, \quad \forall \alpha^{0} \in \Lambda^{0}$$

$$\tag{40}$$

because of (36), and that:

$$\mathcal{L}_{\underline{v}}\alpha^n = d\iota_{\underline{v}}\alpha^n, \quad \forall \alpha^n \in \Lambda^n \tag{41}$$

because of (29).

#### **3 DISCRETE DIFFERENTIAL GEOMETRY**

The process of discretizing a physical process modeled by a differential equation involves two distinct, although connected since both influence each other, steps: the discretization of the physical quantities and the discretization of the operators that establish the relations between them and with the physical space-time in which they lie. One will start by introducing the discretization of differential forms and then will introduce the discrete exterior derivative, a purely topological operator, and then the discrete Hodge-\* and metric dependent operators. It will become clear that the discretization of the exterior derivative, being of topological nature, can be done exactly with no error involved, contrasting with all metric dependent operators that due to their local nature can only be approximated. Hence the crucial point of a good discretization scheme resides in the way in which the metric dependent operators are approximated.

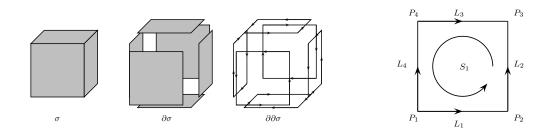


Figure 1: Left: the boundary of a cube and the corresponding boundaries of each face of the boundary of the cube. Right: orientation of a surface and of the lines that constitute its boundary,  $L_3$  and  $L_4$  have an opposite orientation to the one of the boundary of  $S_1$ , induced by the orientation of  $S_1$ , and  $L_1$  and  $L_2$  have the same orientation of the one of the boundary of  $S_1$ , induced by the orientation of  $S_1$ .

### 3.1 Discrete differential forms and Discrete exterior derivative

The process of discretization of physical quantities, hence differential forms, can be seen simply as a choice of a finite set of degrees of freedom (or samples), that are used to represent a continuous physical quantity. With this finite representation one can easily represent the physical quantities as finite dimensional column vectors, and all linear operators acting on them as matrices. Although, in principle, the choice of degrees of freedom is arbitrary, it turns out that some choices are be better than others. This choice explicitly determines how the discrete operators are. Here, one will try to give a motivation for the choice made for the degrees of freedom used to discretize differential forms, avoiding as much as possible an *ad hoc* introduction.

It was stated before, see subsection 2.4, that k-forms are naturally integrated over k-dimensional manifolds. Another property that was introduced was Stokes' theorem:

$$\int_{\Omega^{k+1}} d\alpha^k = \int_{\partial\Omega^{k+1}} \alpha^k \tag{42}$$

This, again, stresses the important role that integration plays in differential forms and their relation to differentiation. Let one consider a 3-dimensional space, say  $\mathbb{R}^3$ . See figure (1).

Here, Stokes' theorem for 0-forms becomes:

$$\int_{\Omega^1} d\alpha^0 = \alpha^0(P_2) - \alpha^0(P_1), \quad \forall \alpha^0 \in \Lambda^0$$
(43)

with  $\Omega^1$  a curve in  $\mathbb{R}^3$ , starting at point  $P_1$  and ending at point  $P_2$ . Now, for the case of 1-forms, Stokes' theorem becomes:

$$\int_{\Omega^2} d\alpha^1 = \int_{\partial\Omega^2} d\alpha^1, \quad \forall \alpha^1 \in \Lambda^1$$
(44)

with  $\Omega^2$  a surface in  $\mathbb{R}^3$ . Now, consider that  $\Omega^2$  is a square in the *xy*-plane, whose bottom, top, left and right boundaries are  $\partial \Omega_{y-}^2$ ,  $\partial \Omega_{y+}^2$ ,  $\partial \Omega_{x-}^2$ ,  $\partial \Omega_{x+}^2$ , and are oriented in the positive direction of the axis., then:

$$\int_{\Omega^2} d\alpha^1 = \int_{\partial\Omega^2} d\alpha^1 = \int_{\partial\Omega^2_{y_-}} d\alpha^1 - \int_{\partial\Omega^2_{y_+}} d\alpha^1 + \int_{\partial\Omega^2_{x_+}} d\alpha^1 - \int_{\partial\Omega^2_{x_-}} d\alpha^1, \quad \forall \alpha^1 \in \Lambda^1 \quad (45)$$

The same can be done for a 2-form, if with  $\Omega^3$  in this case is a cube with faces parallel to the coordinate axis, denoted by  $\partial \Omega^3_{x+}$ ,  $\partial \Omega^3_{x-}$ ,  $\partial \Omega^3_{y+}$ ,  $\partial \Omega^3_{y-}$ ,  $\partial \Omega^3_{z+}$  and  $\partial \Omega^3_{z-}$ , and oriented in the positive direction of the axis, then:

$$\int_{\Omega^3} d\alpha^2 = \int_{\partial\Omega^3} \alpha^2 = \int_{\partial\Omega^3_{x-}} \alpha^2 - \int_{\partial\Omega^3_{x+}} \alpha^2 + \int_{\partial\Omega^3_{y-}} \alpha^2 - \int_{\partial\Omega^3_{y+}} \alpha^2 + \int_{\partial\Omega^3_{z-}} \alpha^2 - \int_{\partial\Omega^3_{z+}} \alpha^2 \quad (46)$$

valid for all  $\alpha^2 \in \Lambda^2$ . For a 3-form, since  $d\alpha^3 := 0$ , in any 3-dimensional manifold, (29), then its integral must also be zero.

Having in mind these last four equations, it makes sense, although not a trivial step, to use as degrees of freedom for k-forms their integrals over a set of k-dimensional manifolds. In this way, 0-forms can be represented by their values at a set of points, 1-forms by their line integrals over a set of curves, 2-forms by their surface integrals over a set of surfaces, 3-forms by their volume integral over a set of volumes, and so on. This not only makes sense but also is compatible with the exterior derivative and Stokes' theorem.

The choice of geometrical objects where to sample the differential forms, although endowed with some freedom is not completely arbitrary. Again, using Stokes' theorem, one sees that the exterior differentiation combined with integration relate geometrical objects with their boundary. Hence it is necessary to construct the geometrical objects such that the set of geometrical objects on the boundary of each geometrical object  $\Omega^k$ , is contained in the set of geometrical objects  $\Omega^{k-1}$ , that is:

$$\forall \Omega^k \in C^k \Rightarrow \partial \Omega^k_i \subseteq C^{k-1} \tag{47}$$

where  $C^k$  is the set of all geometrical objects of k-dimension taken as integration domains for the discretization of k-forms. This is satisfied by a *tesselation*<sup>8</sup> of the space-time, in which the phenomena occur, with *convex polytopes*<sup>8</sup>, that is, a usual mesh in which nodes, edges, faces, volumes, and so on, now all play an equivalent role.

With this introduction, one can define the discretization, or reduction, operator,  $\mathcal{R}^k$ , of a k-form, given a tesselation, T, of space-time:

$$\mathcal{R}^k : \Lambda^k \to \mathbb{R}^m \tag{48}$$

where m is the number of k-dimensional geometrical objects in the tesselation T. In this way:

$$\mathcal{R}^{k}(\alpha^{k}) = \boldsymbol{v}^{k} = [v_{i}] = \left[ \int_{\Omega_{i}^{k}} \alpha^{k} \right], \quad \boldsymbol{v}^{k} \in \mathbb{R}^{m}, \quad \Omega_{i}^{k} \in T$$

$$(49)$$

In this way it is possible to construct an exterior differentiation that exactly represents the continuous one, if done properly. Let  $\beta^k \in \Lambda^k$  and  $\alpha^{k+1} \in \Lambda^{k+1}$  be such that  $d\beta^k = \alpha^{k+1}$ . Moreover, let their discretizations be  $\mathcal{R}^k(\beta^k) = \mathbf{b}^k$  and  $\mathcal{R}^k(\alpha^{k+1}) = \mathcal{R}^k(d\beta^k) = \mathbf{a}^{k+1}$  then one wishes to have that the discrete exterior derivative acting on discrete k-forms,  $D^k = [D_{ij}^k]$ , to exactly satisfy:

$$D^{k}\mathcal{R}^{k}(\beta^{k}) = \mathcal{R}^{k+1}(d\beta^{k}) = \mathcal{R}^{k+1}(\alpha^{k+1})$$
(50)

Which is, in terms of the discretized forms:

$$D^k \boldsymbol{b}^k = \boldsymbol{a}^{k+1} \tag{51}$$

But, using Stokes' theorem, (42):

$$\int_{\Omega_i^{k+1}} \alpha^{k+1} = \int_{\partial \Omega_i^{k+1}} d\beta^k = \int_{\partial \Omega_i^{k+1}} \beta^k = \sum_j c_{ji}^{k+1} \int_{\Omega_j^k \in \partial \Omega_i^{k+1}} \beta^k$$
(52)

where  $c_{ji}^{k+1}$  are coefficients that relate the orientation of the boundary of the geometrical object  $\Omega_i^{k+1}$  to the geometrical object  $\Omega_j^k$ , -1 if they have opposite orientations, 1 if they have the same orientation and 0 if  $\Omega_j^k \notin \partial \Omega_i^{k+1}$ . One can define a matrix of these coefficients,  $C^{k+1}$ , as  $C^{k+1} = [c_{ij}^{k+1}]$ . In this way, combining the definition of the discretization of a k-form, (49), with (52), yields:

$$a^{k+1} = (C^{k+1})^t b^k$$
(53)

where  $(C^{k+1})^t$  is the transpose of the matrix  $C^{k+1}$ . Combining (51) with (53), follows directly that:

$$D^{k} = (C^{k+1})^{t} (54)$$

This relation is very important since it can be shown<sup>9,14,15</sup> that  $C^{k+1} = \partial^{k+1}$ , with  $\partial^{k+1}$  the discrete boundary operator, that acts on geometrical objects of dimension k+1, hence, the formal discrete duality pairing can be made:

$$\langle D^k \boldsymbol{a}^k, \Omega^{k+1} \rangle = \langle \boldsymbol{a}^k, \partial^{k+1} \Omega^{k+1} \rangle$$
 (55)

since  $D^k = (\partial^{k+1})^t$ . This mimics exactly the continuous one:

$$\langle d\alpha^k, \Omega^{k+1} \rangle := \int_{\Omega^{k+1}} d\alpha^k = \int_{\partial \Omega^{k+1}} \alpha^k := \langle \alpha^k, \partial \Omega^{k+1} \rangle$$
(56)

#### 3.2 Discrete metric dependent operators

As stated previously, metric dependent operators are the most difficult to discretize and are the ones that yield all approximations the scheme will contain. In this section one will introduce a method to discretize any metric dependent operator. The idea behind this method lies in the reconstruction of an *approximation* of the continuous differential form from the discretized one. One stresses *approximation* since, upon discretization, part of the information contained in the original continuous differential form is lost and cannot be retrieved since the discretization is nothing but a projection operator from a higher dimensional space onto a smaller dimensional space. The reconstruction process is, essentially, an histopolation<sup>11,18</sup>,  $\mathcal{I}_p^k$ , that takes the discrete degrees of freedom and maps them into a continuous, polynomial of order p, differential form:

$$\mathcal{I}_p^k : \mathbb{R}^m \mapsto \Lambda_p^k \subset \Lambda^k \tag{57}$$

that acts on discrete differential k-forms,  $\boldsymbol{a}^k \in \mathbb{R}^m$  in the following way:

$$\mathcal{I}_p^k(\boldsymbol{a}^k) := \sum_i a_i^k \epsilon_i^{k,p}(x^1, \dots, x^n)$$
(58)

Where  $\epsilon_i^{k,p}$  are k-form basis functions<sup>11,18</sup> of order p. For a 0-form, the reconstruction operator  $\mathcal{I}_p^0$  is the usual nodal interpolation operator of order p. For higher rank forms, they are designated in the literature as edge basis functions<sup>11</sup>.

Having introduced the p order reconstruction operator of k-forms,  $\mathcal{I}_p^k$ , the procedure to discretize any metric dependent operator, or combination of them, is done in the following way. Reconstruct the differential form using the reconstruction operator, then find the discrete version of the operator that minimizes the difference in the  $L^2$  norm, (33). Let us consider an example arbitrary metric dependent operator,  $\bigstar$ , and its discrete version,  $S_p^k = [S_{ij}^{k,p}]$ , which as already stated, can be any combination of operators, for example  $\star$ ,  $\iota_{\underline{v}}$  or  $\iota_{\underline{v}} \star$ :

$$\bigstar : \Lambda^k \mapsto \Lambda^q, \quad S_p^k : \mathbb{R}^n \mapsto \mathbb{R}^m \tag{59}$$

We have, for  $\alpha^k = \mathcal{I}_p^k(\boldsymbol{a}^k)$  and  $\beta^k = \mathcal{I}_p^q(\boldsymbol{b}^q)$ , in the continuous level and in the discrete level:

$$\alpha^k := \bigstar \beta^q, \qquad \boldsymbol{a}^k \approx S_p^q \boldsymbol{b}^q \tag{60}$$

Hence,  $S_p^k$  is found by setting to zero the following difference in the  $L^2$  inner product:

$$\langle \mathcal{I}_{p}^{k}(\boldsymbol{a}^{k}) - \bigstar \mathcal{I}_{p}^{q}(\boldsymbol{b}^{q}), \epsilon_{j}^{k,p} \rangle = 0, \quad \forall \epsilon_{j}^{k,p}, \forall \boldsymbol{b}^{q}$$
 (61)

Which, using (60) gives:

$$\langle \mathcal{I}_{p}^{k}(S_{p}^{q}\boldsymbol{b}^{q}) - \bigstar \mathcal{I}_{p}^{q}(\boldsymbol{b}^{q}), \epsilon_{j}^{k,p} \rangle = 0, \quad \forall \epsilon_{j}^{k,p}, \forall \boldsymbol{b}^{q}$$
(62)

And using the definition of the reconstruction operator, (58), gives:

$$\left\langle \sum_{i,l} S_{il}^{q,p} b_l^q \epsilon_i^{k,p} - \bigstar \left( \sum_l b_l^q \epsilon_l^{q,p} \right), \epsilon_j^{k,p} \right\rangle = 0, \quad \forall \epsilon_j^{k,p}, \forall \boldsymbol{b}^q$$
(63)

Taking all constants outside, by linearity of the  $L^2$  inner product, and noting that, by linearity of  $\bigstar$  operator, one can interchange constants with  $\bigstar$ :

$$\sum_{i,l} S_{il}^{q,p} b_l^q \langle \epsilon_i^{k,p}, \epsilon_j^{k,p} \rangle - \sum_l b_l^q \langle \bigstar \epsilon_l^{q,p}, \epsilon_j^{k,p} \rangle = 0, \quad \forall \epsilon_j^{k,p}, \forall \boldsymbol{b}^q$$
(64)

In matrix notation this is:

$$E_p^k S_p^q \boldsymbol{b}^q - (\overline{E}_p^{q,k})^t \boldsymbol{b}^q = 0, \quad \forall \boldsymbol{b}^q$$
(65)

Where,  $E_p^k = (E_p^k)^t = [\langle \epsilon_i^{k,p}, \epsilon_j^{k,p} \rangle]$  and  $\overline{E}_p^{q,k} = [\langle \bigstar \epsilon_l^{q,p}, \epsilon_j^{k,p} \rangle]$ . Which implies that:

$$S_{p}^{q} = (E_{p}^{k})^{-1} (\overline{E}_{p}^{q,k})^{t}$$
(66)

## 4 ADVECTION EQUATION

#### 4.1 Continuous formulation

As mentioned in Section 1, the advection equation in vector notation can be represented in the following way:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\boldsymbol{v}\rho) = 0 \quad (\boldsymbol{x}, t) \in \Omega \times [0, T], \quad \rho(t, \partial \Omega_{\rm in}) = \rho_b(t), \quad \rho(0, \boldsymbol{x}) = \rho_0(\boldsymbol{x}) \tag{67}$$

This is the differential formulation of the advection equation of the scalar quantity  $\rho$  by the flow  $\boldsymbol{v}$ . It is possible to integrate it in space and time and obtain the equivalent integral formulation, valid for any space-time volume  $\overline{\Omega} \subseteq \Omega \times [0, T]$ :

$$\int_{\overline{\Omega}} \frac{\partial \rho}{\partial t} \, dV dt + \int_{\overline{\Omega}} \nabla \cdot (\boldsymbol{v}\rho) \, dV dt = 0, \quad \forall \overline{\Omega} \tag{68}$$

The divergence operator  $\nabla \cdot$ , which is space like only, can be extended to a space-time divergence operator,  $\overline{\nabla} \cdot$ , in a straightforward way:  $\overline{\nabla} \cdot := (\frac{\partial}{\partial x^1}, \ldots, \frac{\partial}{\partial x^n}, \frac{\partial}{\partial t}) \cdot$ . In this way, introducing the space-time current vector,  $\boldsymbol{J} := (\boldsymbol{v}\rho, \rho)$ , one can express (68) in the following form:

$$\int_{\overline{\Omega}} \overline{\nabla} \cdot \boldsymbol{J} \, dV dt = 0, \quad \forall \overline{\Omega} \tag{69}$$

Using Gauss's theorem, this space-time volume integral can be expressed as a flux integral over the space and time boundaries:

$$\int_{\partial \overline{\Omega}} \boldsymbol{J} \cdot \boldsymbol{n} \, dS = 0, \quad \forall \overline{\Omega} \subseteq \Omega \times [0, T]$$
(70)

This space-time formulation simply states that the content of the quantity advected, at any time instant,  $t + \Delta t$ , is equal to what was there at time instant t plus the balance between what flowed into and out of the domain.

Using differential geometry, an equivalent equation is derived, rendering an appropriate discretization scheme since all physical quantities are associated to proper differential forms and, as was seen previously in Section 3, there is a direct discrete analogue to each differential form and each operator. If one introduces the space-time velocity vector  $\underline{v} := v^i \partial_i + \partial_t$ , and the space-time scalar quantity 0-form,  $\rho^0 = \rho$ , then the following equation is equivalent to (67):

$$\mathcal{L}_v \star \rho^0 = 0, \quad \forall \overline{\Omega} \subseteq \Omega \times [0, T] \tag{71}$$

It is not immediate that this equation is the analogous of (67). It seems unnatural to start with a 0-form and then apply the Hodge- $\star$  to it: why not start with a volume form directly? The reason being the fact that physically  $\rho^0$ , the space-time 0-form, is not the usual density  $\rho$  that is naturally integrated in space, although related in the following way. As pointed previously, the space-time velocity,  $\underline{v}$ , contains a space-like component and a time-like component. In this way, when one usually refers to zero velocity in fact one moves in space-time with the velocity  $\underline{v} = \partial_t$ . Hence the usual density, naturally integrated in space, in terms of space-time differential forms, is a time-like flux, that is, a space-like (n)-form in the (n+1)-dimensional space-time, the space-like components of the mass current form,  $j^n$ . This mass current form is given by  $\star(\rho^0 \wedge \underline{v}^{\flat})$  which can be rewritten as<sup>6</sup>  $\iota_{\underline{v}} \star \rho^0$ . The statement that  $j^n$  should be conserved, leads directly to the conservation equation:

$$dj^n = d\iota_{\underline{v}} \star \rho^0 \tag{72}$$

This, noting that  $\star \rho^0$  is an (n + 1)-form in space-time and hence (41) holds, lead directly to (71). This is a common formulation of advection in relativistic hydrodynamics<sup>23</sup>. Nevertheless, an interesting point that certainly deserves further investigation is the Lie advection of the volume form,  $\rho^{n+1} = \star \rho^0$ , directly. To show that (71) is in fact equivalent to (67) one just needs to use Cartan's magic formula, (39), the definition of the Hodge- $\star$ operator, (32), and to use the relation  $d \star \alpha^0 = 0$ , valid for all  $\alpha^0 \in \Lambda^0$ , obtaining:

$$\mathcal{L}_{\underline{v}} \star \rho^{0} = d\iota_{\underline{v}} \star \rho^{0} = d\iota_{\underline{v}} \rho \, d\theta \wedge dt = 0 \tag{73}$$

where  $\theta := dx^1 \wedge \ldots \wedge dx^n$  is the space-like volume form. Using the definition of interior product, (35) and (37):

$$\mathcal{L}_{\underline{v}} \star \rho^{0} = d \left( \rho v^{i} d\theta |_{i} \wedge dt + (-1)^{n} \rho d\theta \right) = 0$$
(74)

where  $\theta|_i := dx^1 \wedge \ldots \wedge (dx^i) \wedge \ldots \wedge dx^n$ ,  $(dx^i)$  meaning that the term  $dx^i$  does not appear. It is clear, see (38), that  $\mathcal{L}_{\underline{v}} \star \rho^0$  is a space-time (n+1)-form, that is, a space-time volume form, hence naturally integrated over a space-time manifold of dimension n+1,  $\overline{\Omega}$ :

$$\int_{\overline{\Omega}} \mathcal{L}_{\underline{v}} \star \rho^0 = \int_{\overline{\Omega}} d\left(\rho v^i d\theta|_i \wedge dt + (-1)^n \rho d\theta\right) = 0$$
(75)

Which is simply a formulation of (69) in terms of concepts of differential geometry. Using the generalized Stokes theorem, (30), one can write:

$$\int_{\overline{\Omega}} \mathcal{L}_{\underline{v}} \star \rho^0 = \int_{\partial \overline{\Omega}} \rho v^i d\theta |_i \wedge dt + (-1)^n \rho d\theta = 0$$
(76)

Which, again, is simply a formulation of (70) in terms of concepts of differential geometry. In this way, solving (69) or (70) is equivalent to solving (67), with the advantage that a proper discretization scheme is straightforwardly obtained from Section 3. This will be presented next.

#### 4.2 Discrete formulation

For the implementation of the discretization of the advection equation one takes its differential form formulation, (75) identical to (72). With this, one has two distinct, but related, physical quantities:  $\rho^0$ , a space-time 0-form, and mass current  $j^1$  a space-time (*n*)-form, if space has dimension *n*. These two physical quantities are related by a metric dependent operator:  $\iota_{\underline{v}}\star$ . And an additional topological relation that states that the mass current,  $j^n$ , has exterior derivative, *d*, identical to zero. Hence, following the path presented in Section 3, one needs to discretize one 1-form, one *n*-form and two operators, one metric dependent,  $\iota_v\star$  and another an exterior derivative, metric independent.

For the discretization of the differential forms, one uses nodal basis functions of order p for the zero form, and edge basis functions of rank n and order p for the n-form, hence defining their degrees of freedom as point evaluations, 0-form, and as n-dimensional flux integrals,:

$$\mathcal{R}^{k}(\rho^{0}) = \boldsymbol{\rho}^{0}, \quad \mathcal{R}^{k}(j^{n}) = \boldsymbol{j}^{n}$$
(77)

For the exterior derivative, (54) is used. As for  $\iota_{\underline{v}}\star$ , its discrete counterpart,  $S_p^q$  is given by:

$$S_p^0 = (E_p^n)^{-1} (\overline{E}_p^{n,0})^t$$
(78)

Where,  $E_p^n = (E_p^n)^t = [\langle \epsilon_i^{n,p}, \epsilon_j^{n,p} \rangle]$  and  $\overline{E}_p^{0,k} = [\langle \iota_{\underline{v}} \star \epsilon_l^{0,p}, \epsilon_j^{n,p} \rangle]$ . This will yield the following system of equations:

$$\begin{pmatrix} E_p^n & (\overline{E}_p^{n,0})^t \\ D^n & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{j}^1 \\ \boldsymbol{\rho}^0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
(79)

#### 4.3 Numerical results and discussion of results

As a preliminary study of this numerical scheme, it was applied, for (1+1)-space-time, to the linear advection in a steady and uniform velocity field,  $\underline{v} = \partial_x + \partial_t$ , over the time intervals, T = 8.0s, 95s, for cosine hill and square wave initial condition, periodic boundary conditions spatial length,  $L_x = 5.0m$ . These computations where performed for four different CFL numbers: 0.8, 1.0, 1.8 and 9.0, obtaining the following results: One can see, observing figure (2), that the numerical scheme presented behaves very well for a

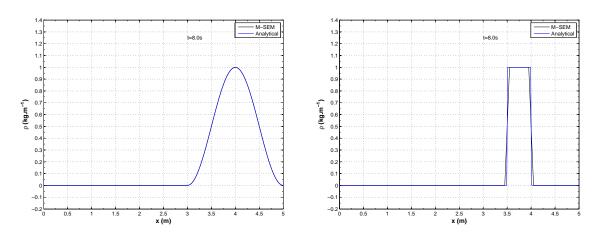


Figure 2: Left: cosine hill advection. Right: square wave advection. Both: CFL=1.0, p=1,  $\Delta x=0.05$ ,  $\Delta t=0.05$ .

CFL=1, not dissipating energy and preserving the speed and shape of the traveling wave. Observing figure (3) it is possible to state that the scheme behaves well for the advection of the cosine hill, but for a square wave spurious oscillations appear. An interesting point is the fact that this oscillations do not increase in time, they are kept with a bounded amplitude. This effect was noticed in all discontinuous traveling waves tested. Looking at figure (4) it is possible to see that the scheme preserves mass exactly, as expected, since the conservation of mass is explicitly introduced in the scheme. A surprising fact is the almost conservation of energy, which oscillates but does not diverge from the initial value at t = 0.

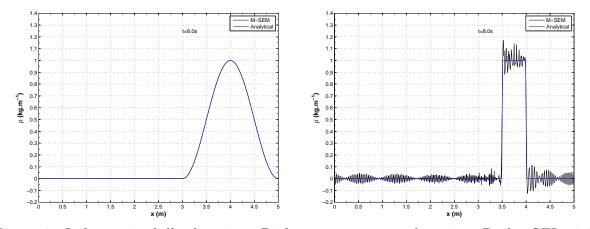


Figure 3: Left: cosine hill advection. Right: square wave advection. Both: CFL=0.8, p=1,  $\Delta x=0.0521$ ,  $\Delta t=0.0417$ .

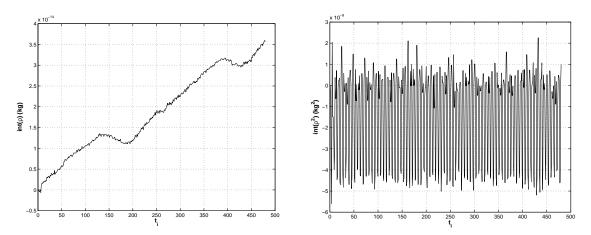


Figure 4: Left: Mass conservation at each time step. Right: Energy conservation at each time step. Both: CFL=0.8, p=5,  $\Delta x=0.1562$ ,  $\Delta t=0.1250$ , advection of a cosine hill.

## 5 CONCLUSIONS

In this work, a mimetic scheme for the solution of the advection equation in spacetime is presented. Taking as a starting point the framework of differential geometry, it is possible to develop a numerical scheme capable of capturing many structural properties of the differential equation that it tries to solve. In doing so, one obtained a reasonably stable scheme that is capable of adequately advecting smooth initial conditions for large time intervals with no dissipation and spurious oscillations. The not so good behaviour of this scheme for discontinuous initial conditions alerts to the possibility of existence of some inconsistencies in the development of the scheme. In this way, further research is to be taken in this direction, given the promising results obtained.

#### 6 ACKNOWLEDGMENTS

The authors would like to acknowledge Foundation for Science and Technology (Portugal) for the funding given by the PhD grant SFRH/BD/36093/2007.

#### References

- [1] R. Abraham, J. E. Marsden, and T. Ratiu. *Manifolds, Tensor Analysis, and Appli*cations, volume 75 of Applied Mathematical Sciences. Springer, 2001.
- [2] A. Bossavit. On the geometry of electromagnetism. Journal of the Japanese Society of Applied Electromagnetics and Mechanics, 6:17–28 (no 1), 114–23 (no 2), 233–40 (no 3), 318–26 (no 4), 1998.
- [3] A. Bossavit. Computational electromagnetism and geometry. Journal of the Japanese Society of Applied Electromagnetics and Mechanics, 7, 8:150–9 (no 1), 294–301 (no 2), 401–408 (no 3), 102–109 (no 4), 203–209 (no 5), 372–377 (no 6), 1999, 2000.

- [4] A. Bossavit. Extrusion, contraction: their discretization via whitney forms. The International Journal for Computation and Mathematics in the Electrical and Electronic Engineering, 22(2):470–480, 2003.
- [5] M. Bouman, A. Palha, J. Kreeft, and M. Gerritsma. A conservative spectral element method for arbitrary domains. *Proceedings of ICOSAHOM2009*, 2010.
- [6] W. Burke. Applied differential geometry. Cambridge Univ Pr, 1985.
- [7] J. B. Conway. A course in functional analysis. Graduate texts in mathematics. Springer, 1994.
- [8] H. Coxeter and H. Coxeter. *Regular polytopes*. Dover Pubns, 1973.
- M. Desbrun, A. Hirani, M. Leok, and J. Marsden. Discrete exterior calculus. Arxiv preprint math/0508341, 2005.
- [10] H. Flanders. *Differential forms with applications to the physical sciences*. Dover publications, 1989.
- [11] M. Gerritsma. Edge functions for spectral element methods. Submitted to the proceedings of ICOSAHOM 2009 (this issue), 2010.
- [12] B.-Y. Hou and B.-Y. Hou. Differential geometry for physicists, volume 6 of Advanced series on theoretical physical science. World Scientific, 1997.
- [13] C. J. Isham. Modern differential geometry for physicists, volume 61 of Lecture Notes in Physics. World Scientific, 2001.
- [14] J. J. Kreeft, A. Palha, and M. I. Gerritsma. Mimetic spectral element method for generalized convection-diffusion problems. *Proceedings of ECCOMAS2010, this issue*, 2010.
- [15] C. Mattiussi. The finite volume, finite element, and finite difference methods as numerical methods for physical field problems. Advances in Imaging and electron physics, 113:1–147, 2000.
- [16] P. Mullen, A. McKenzie, D. Pavlov, L. Durant, Y. Tong, E. Kanso, J. Marsden, and M. Desbrun. Discrete lie advection of differential forms. Arxiv preprint arXiv:0912.1177, 2009.
- [17] A. Palha and M. Gerritsma. Spectral element approximation of the hodge-★ operator in curved elements. Proceedings of ICOSAHOM2009, 2010.

- [18] N. Robidoux. Polynomial histopolation, superconvergent degrees of freedom, and pseudospectral discrete hodge operators. Unpublished: http://www.cs.laurentian.ca/nrobidoux/prints/super/histogram.pdf, 2008.
- [19] M. Shigeyuki. Geometry of differential forms, volume 201 of Translations of mathematical monographs. American mathematical society, 2001.
- [20] M. Spivak. *Calculus on manifolds*. Perseus Books, 1998.
- [21] E. Tonti. On the formal structure of physical theories. preprint of the Italian National Research Council, 1975.
- [22] J. Volker and P. Knobloch. On spurious oscillations at layers diminishing (sold) methods for convection-diffusion equations: Part i - a review. *Computer methods in* applied mechanics and engineering, 196(17-20):2197-2215, March 2006.
- [23] J. Wilson and G. Mathews. *Relativistic numerical hydrodynamics*. Cambridge Univ Pr, 2003.