



Mimetic Methods on Measure Chains

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Abstract—We introduce the divergence and the gradient for functions defined on a measure chain, and this includes as special cases both continuous derivatives and discrete forward differences. It is shown that in one dimension, subject to Dirichlet boundary conditions, the divergence and the gradient are negative adjoints of each other and that the divergence of the gradient is negative semidefinite. These are well-known results in the continuous theory, and hence, mimic those properties also for the case of a general measure chain. © 2001 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

Mimetic discretizations of differential operators are discretizations that preserve many of the fundamental properties of the continuum differential operators. Certainly any reasonable discretization will preserve some of the continuum properties, so really the goal is to maximize the number of properties that are preserved, or if this is not possible, to clearly understand what tradeoffs are required in preserving most of the properties (see [1–3]). In this work, preserving means to preserve exactly, not approximately, although it would be natural to generalize this work to preserving some properties at higher order than the basic discretization. A validation of mimetic differential operators is presented here using the calculus of *time scales* (or *measure chains*). This calculus has been introduced by Aulbach and Hilger [4] (see also [5–7]) in order to unify continuous and discrete analysis. Hence, all the results that we prove below ensure mimetism as they are shown in a general setting containing both the continuous and the discrete as special cases. But not only does this approach contain the continuous and the discrete, but it also contains mixtures of those or cases in between.

One of the most important types of properties to preserve are *conservation* laws. This naturally leads to the classical finite-volume methods. In the continuum, proofs of the conservation laws rely on the potential, divergence, and Stokes theorems from vector calculus, so the preservation of these theorems is very important. To even state these theorems, we need not only the notion

of a derivative on a time scale, but also the notion of an integral on such a time scale, as well as versions of the chain rule and substitution rule and derivative of the inverse function. All these tools are developed below.

Mimetic methods are important and will become even more important for simulations, especially where the physical material properties are not smoothly varying, the solution is rapidly varying, the grid used for the discretization is not regular, or for long-time simulations. Mimetic discretizations have a life of their own. That is, it is not necessary to view them as a discretization of a continuum system. We only need to do this when we want to know if the discrete system approximates some continuum system. So the crucial points are summation formulas. In summary, we will say that a discretization of the first derivative and the one-dimensional integral are mimetic if there are analogs of the Fundamental Theorem and the integration by parts formula, that are exact. Either of these results imply global conservation, and local conservation implies that the null space of the derivative is a constant.

The paper is organized as follows. The next section contains an introduction into the time scales calculus as developed by Aulbach and Hilger and features some basic and well-known results from this calculus, such as, e.g., the product rule for the derivative of the product of two functions on a measure chain. Section 3 contains further results on the time scales calculus that have been developed in order to show the main results of this paper, such as, e.g., the chain rule and the substitution rule. Finally, in Section 4 we prove the main results of this paper concerning mimetic properties of the divergence and the gradient on time scales. Subject to Dirichlet boundary conditions, we obtain that the operators div and grad are negative adjoints of each other and that the operator div grad is negative semidefinite. It certainly would be useful to generalize those properties to higher dimensions, but presently such a generalization remains open.

2. THE TIME SCALES CALCULUS

The calculus of time scales has been introduced by Hilger [7] in order to unify discrete and continuous analysis. A time scale \mathbb{T} is an arbitrary closed subset of the reals \mathbb{R} , and in this paper we assume that it is bounded, too (hence, \mathbb{T} is compact). The time scale induces so-called jump operators σ and ρ by

$$\sigma(t) = \inf\{s \in \mathbb{T} : s > t\} \quad \text{and} \quad \rho(t) = \sup\{s \in \mathbb{T} : s < t\}$$

(supplemented by $\inf \emptyset = \sup \mathbb{T}$ and $\sup \emptyset = \inf \mathbb{T}$). Note that both σ and ρ map \mathbb{T} into \mathbb{T} . The so-called graininess μ is now defined by $\mu(t) = \sigma(t) - t$. It maps elements of \mathbb{T} into the set of nonnegative real numbers. For a function $f : \mathbb{T} \rightarrow \mathbb{R}$ we may define the derivative f^Δ as follows. Let $t \in \mathbb{T}$. If there exists a number $\alpha \in \mathbb{R}$ such that for all $\varepsilon > 0$ there exists a neighborhood U of t with

$$|f(\sigma(t)) - f(s) - \alpha(\sigma(t) - s)| \leq \varepsilon|\sigma(t) - s|, \quad \text{for all } s \in U,$$

then f is said to be differentiable at t , and we call α the derivative of f at t and denote it by $f^\Delta(t)$. Basic facts of this derivative are collected in the following lemma. We put $f^\sigma = f \circ \sigma$.

LEMMA 2.1. PROPERTIES OF THE DERIVATIVE.

- If f is differentiable at t , then it is continuous at t .
- If f is differentiable at t , then the formula $f^\sigma = f + \mu f^\Delta$ holds at t .
- If both f and g are differentiable at t , then the product fg is also differentiable at t , and the formula $(fg)^\Delta = f^\Delta g + f^\sigma g^\Delta$ holds at t .

If a function f on \mathbb{T} possesses an antiderivative F , i.e., $F^\Delta = f$, then we can define an integral of f by the formula

$$\int_a^b f(t) \Delta t = F(b) - F(a), \quad \text{where } a, b \in \mathbb{T}.$$

The fundamental existence result then reads as follows.

LEMMA 2.2. *If f is an rd-continuous function on \mathbb{T} , then it possesses an antiderivative.*

Above, we call a function rd-continuous provided it is continuous in right-dense points (i.e., points t with $\sigma(t) = t$; other points are called right-scattered) and has a left-sided limit in left-dense points (i.e., points t with $\rho(t) = t$; other points are called left-scattered).

Crucial for the results presented below is the integration by parts formula, which follows directly from the above product rule and the definition of the integral.

LEMMA 2.3. INTEGRATION BY PARTS. *Suppose $f^\Delta g$ and $f^\sigma g^\Delta$ are rd-continuous. Then*

$$\int_a^b (f^\Delta g)(t) \Delta t = f(b)g(b) - f(a)g(a) - \int_a^b (f^\sigma g^\Delta)(t) \Delta t.$$

EXAMPLE 2.1. The two most popular examples of a measure chain are $\mathbb{T} = \mathbb{R}$ and $\mathbb{T} = \mathbb{Z}$. In the first case, we have

$$\sigma(t) = \rho(t) = t \quad \text{and} \quad \mu(t) \equiv 0$$

and the derivative f^Δ of a function f is simply f' if it exists. In this case, rd-continuity is the same as continuity as every point is left-dense and right-dense at the same time. For continuous functions the integral exists, and it is the usual integral from calculus. Next, for the case $\mathbb{T} = \mathbb{Z}$, we have

$$\sigma(t) = t + 1, \quad \rho(t) = t - 1, \quad \text{and} \quad \mu(t) \equiv 1.$$

The derivative f^Δ of a function f is now Δf , where Δ is the usual forward difference operator defined by $\Delta f(k) = f(k+1) - f(k)$. In this case, every function is rd-continuous, and the integral from a to b , where a and b are integers with $a < b$, is simply the sum of $f(k)$ for k from a to $b - 1$.

EXAMPLE 2.2. Other examples of time scales are

$$h\mathbb{Z} = \{hk : k \in \mathbb{Z}\},$$

$$q^{\mathbb{Z}} = \{q^k : k \in \mathbb{Z}\} \cup \{0\}, \quad \text{for some } q > 1$$

(which produces so-called q -difference equations),

$$\mathbb{N}^2 = \{k^2 : k \in \mathbb{N}\}, \left\{ \sum_{k=1}^n \frac{1}{k} : n \in \mathbb{N} \right\}, \bigcup_{k \in \mathbb{Z}} [2k, 2k + 1],$$

or the Cantor set.

3. THE CHAIN RULE

Let \mathbb{T} be a time scale and $\nu : \mathbb{T} \rightarrow \mathbb{R}$ be a strictly increasing function such that $\tilde{\mathbb{T}} = \nu(\mathbb{T})$ is also a time scale so that $\nu \circ \sigma = \tilde{\sigma} \circ \nu$. We put $a = \min \mathbb{T}$ and $b = \max \mathbb{T}$, and hence, $\min \nu(\mathbb{T}) = \nu(a)$ and $\max \nu(\mathbb{T}) = \nu(b)$. Let $w : \tilde{\mathbb{T}} \rightarrow \mathbb{R}$.

THEOREM 3.1. CHAIN RULE. *If $\nu^\Delta(t)$ and $w^{\tilde{\Delta}}(\nu(t))$ exist for $t \in \mathbb{T}^\kappa$, then at t*

$$(w \circ \nu)^\Delta = (w^{\tilde{\Delta}} \circ \nu) \nu^\Delta.$$

PROOF. Let $\varepsilon > 0$. Define $\varepsilon^* = \varepsilon[1 + |\nu^\Delta(t)| + |w^{\tilde{\Delta}}(\nu(t))|]^{-1}$, where $\varepsilon^* \in (0, 1)$ without loss of generality. According to the assumptions, there exist neighborhoods \mathcal{N}_1 of t and \mathcal{N}_2 of $\nu(t)$ such that

$$|\nu(\sigma(t)) - \nu(s) - (\sigma(t) - s)\nu^\Delta(t)| \leq \varepsilon^* |\sigma(t) - s|, \quad \text{for all } s \in \mathcal{N}_1$$

and

$$|w(\tilde{\sigma}(\nu(t))) - w(r) - (\tilde{\sigma}(\nu(t)) - r)w^{\tilde{\Delta}}(\nu(t))| \leq \varepsilon^* |\tilde{\sigma}(\nu(t)) - r|, \quad r \in \mathcal{N}_2.$$

Put $\mathcal{N} = \mathcal{N}_1 \cap \nu^{-1}(\mathcal{N}_2)$ and let $s \in \mathcal{N}$. Then $s \in \mathcal{N}_1$ and $\nu(s) \in \mathcal{N}_2$ and

$$\begin{aligned}
 & \left| w(\nu(\sigma(t))) - w(\nu(s)) - (\sigma(t) - s) \left[w^{\tilde{\Delta}}(\nu(t)) \nu^{\Delta}(t) \right] \right| \\
 &= \left| w(\nu(\sigma(t))) - w(\nu(s)) - (\tilde{\sigma}(\nu(t)) - \nu(s)) w^{\tilde{\Delta}}(\nu(t)) \right. \\
 &\quad \left. + [\tilde{\sigma}(\nu(t)) - \nu(s) - (\sigma(t) - s) \nu^{\Delta}(t)] w^{\tilde{\Delta}}(\nu(t)) \right| \\
 &\leq \varepsilon^* |\tilde{\sigma}(\nu(t)) - \nu(s)| + \varepsilon^* |\sigma(t) - s| \left| w^{\tilde{\Delta}}(\nu(t)) \right| \\
 &\leq \varepsilon^* \left\{ |\tilde{\sigma}(\nu(t)) - \nu(s) - (\sigma(t) - s) \nu^{\Delta}(t)| + |\sigma(t) - s| |\nu^{\Delta}(t)| \right. \\
 &\quad \left. + |\sigma(t) - s| \left| w^{\tilde{\Delta}}(\nu(t)) \right| \right\} \\
 &\leq \varepsilon^* \left\{ \varepsilon^* |\sigma(t) - s| + |\sigma(t) - s| |\nu^{\Delta}(t)| + |\sigma(t) - s| \left| w^{\tilde{\Delta}}(\nu(t)) \right| \right\} \\
 &= \varepsilon^* |\sigma(t) - s| \left\{ \varepsilon^* + |\nu^{\Delta}(t)| + \left| w^{\tilde{\Delta}}(\nu(t)) \right| \right\} \\
 &\leq \varepsilon^* \left\{ 1 + |\nu^{\Delta}(t)| + \left| w^{\tilde{\Delta}}(\nu(t)) \right| \right\} |\sigma(t) - s| \\
 &= \varepsilon |\sigma(t) - s|.
 \end{aligned}$$

This proves the claim. ■

REMARK 3.1. DIFFERENTIATION OF THE INVERSE FUNCTION. In particular, we have with $w = \nu^{-1} : \tilde{\mathbb{T}} \rightarrow \mathbb{T}$

$$\left[(\nu^{-1})^{\tilde{\Delta}} \circ \nu \right] \nu^{\Delta} = 1$$

at points where the occurring derivatives exist.

THEOREM 3.2. SUBSTITUTION. If $f : \mathbb{T} \rightarrow \mathbb{R}$ is an rd-continuous function and ν is differentiable with rd-continuous derivative, then

$$\int_{\mathbb{T}} f(t) \nu^{\Delta}(t) \Delta t = \int_{\tilde{\mathbb{T}}} (f \circ \nu^{-1})(s) \tilde{\Delta} s.$$

PROOF. Since $f\nu^{\Delta}$ is an rd-continuous function, it possesses an antiderivative F by Lemma 2.2, i.e., $F^{\Delta} = f\nu^{\Delta}$, and

$$\begin{aligned}
 \int_{\mathbb{T}} f(t) \nu^{\Delta}(t) \Delta t &= \int_{\mathbb{T}} F^{\Delta}(t) \Delta t \\
 &= F(b) - F(a) \\
 &= (F \circ \nu^{-1})(\nu(b)) - (F \circ \nu^{-1})(\nu(a)) \\
 &= \int_{\tilde{\mathbb{T}}} (F \circ \nu^{-1})^{\tilde{\Delta}}(s) \tilde{\Delta} s \\
 &= \int_{\tilde{\mathbb{T}}} (F^{\Delta} \circ \nu^{-1})(s) (\nu^{-1})^{\tilde{\Delta}}(s) \tilde{\Delta} s \\
 &= \int_{\tilde{\mathbb{T}}} ((f\nu^{\Delta}) \circ \nu^{-1})(s) (\nu^{-1})^{\tilde{\Delta}}(s) \tilde{\Delta} s \\
 &= \int_{\tilde{\mathbb{T}}} (f \circ \nu^{-1})(s) \left[(\nu^{\Delta} \circ \nu^{-1})(\nu^{-1})^{\tilde{\Delta}} \right](s) \tilde{\Delta} s \\
 &= \int_{\tilde{\mathbb{T}}} (f \circ \nu^{-1})(s) \tilde{\Delta} s,
 \end{aligned}$$

where we have used the preceding theorem and remark. ■

4. DIVERGENCE, GRADIENT, AND LAPLACIAN

We now define

$$\langle u, W \rangle_{\mathbb{T}} = \int_{\mathbb{T}} u^\sigma(t)W(t) \Delta t \quad \text{and} \quad \langle w, U \rangle_{\tilde{\mathbb{T}}} = \int_{\tilde{\mathbb{T}}} w(t)U(t) \tilde{\Delta} t$$

and introduce the *divergence* and the *gradient* by

$$\operatorname{div} w = (w \circ \nu)^\Delta \quad \text{and} \quad \operatorname{grad} u = (u \circ \nu^{-1})^{\tilde{\Delta}}.$$

EXAMPLE 4.1. Let us shortly discuss some examples. First, if $\mathbb{T} = [a, b]$ and $\nu(t) = t$, then $\tilde{\mathbb{T}} = [a, b]$ and the two inner products defined above are just

$$\langle u, W \rangle_{\mathbb{T}} = \int_a^b u(t)W(t) dt \quad \text{and} \quad \langle w, U \rangle_{\tilde{\mathbb{T}}} = \int_a^b w(t)U(t) dt,$$

while $\operatorname{div} w = w'$ and $\operatorname{grad} u = u'$ if u and w are differentiable. Next, consider the case $\mathbb{T} = \{a, a + 1, \dots, b\}$, where a and b are integers, and $\nu(t) = t + 1/2$. Now we have $\tilde{\mathbb{T}} = \{a + 1/2, a + 3/2, \dots, b + 1/2\}$, and

$$\langle u, W \rangle_{\mathbb{T}} = \sum_{k=a}^{b-1} u(k + 1)W(k), \quad \langle w, U \rangle_{\tilde{\mathbb{T}}} = \sum_{k=a}^{b-1} w\left(k + \frac{1}{2}\right)U\left(k + \frac{1}{2}\right),$$

while $\operatorname{div} w(k) = w(k + 3/2) - w(k + 1/2)$ and $\operatorname{grad} u(k + 1/2) = u(k + 1) - u(k)$. See [1-3] for a discussion of this case. Finally, if \mathbb{T} is any set of discrete points between a and b , we can use $\nu(t) = (t + \sigma(t))/2$ and obtain the new measure chain $\tilde{\mathbb{T}} = \nu(\mathbb{T})$. Of course the results presented below hold for this example as well.

The main result of this paper reads as follows.

THEOREM 4.1. *Suppose that u and w are differentiable functions on \mathbb{T} and $\tilde{\mathbb{T}}$, respectively. Then*

$$\langle u, \operatorname{div} w \rangle_{\mathbb{T}} + \langle w, \operatorname{grad} u \rangle_{\tilde{\mathbb{T}}} = u(b)w(\nu(b)) - u(a)w(\nu(a)).$$

PROOF. Assume that $f = (w \circ \nu)[(u \circ \nu^{-1})^{\tilde{\Delta}} \circ \nu]$ satisfies the assumptions of the substitution theorem. Then it follows by Theorems 3.1 and 3.2 that

$$\begin{aligned} \int_{\mathbb{T}} [u^\Delta(w \circ \nu)](t) \Delta t &= \int_{\mathbb{T}} \left[((u \circ \nu^{-1}) \circ \nu)^\Delta (w \circ \nu) \right](t) \Delta t \\ &= \int_{\mathbb{T}} \left\{ (w \circ \nu) \left[(u \circ \nu^{-1})^{\tilde{\Delta}} \circ \nu \right] \nu^\Delta \right\}(t) \Delta t \\ &= \int_{\mathbb{T}} (f \nu^\Delta)(t) \Delta t \\ &= \int_{\tilde{\mathbb{T}}} (f \circ \nu^{-1})(t) \tilde{\Delta} t \\ &= \int_{\tilde{\mathbb{T}}} \left[w(u \circ \nu^{-1})^{\tilde{\Delta}} \right](t) \tilde{\Delta} t, \end{aligned}$$

and hence, (use also Lemma 2.3)

$$\begin{aligned} \langle u, \operatorname{div} w \rangle_{\mathbb{T}} + \langle w, \operatorname{grad} u \rangle_{\tilde{\mathbb{T}}} &= \int_{\mathbb{T}} (u^\sigma \operatorname{div} w)(t) \Delta t + \int_{\tilde{\mathbb{T}}} (w \operatorname{grad} u)(t) \tilde{\Delta} t \\ &= \int_{\mathbb{T}} [(u^\sigma(w \circ \nu)^\Delta)](t) \Delta t + \int_{\tilde{\mathbb{T}}} \left[\left(w(u \circ \nu^{-1})^{\tilde{\Delta}} \right) \right](t) \tilde{\Delta} t \end{aligned}$$

$$\begin{aligned}
&= \int_{\mathbb{T}} [u^\sigma(w \circ \nu)^\Delta](t) \Delta t + \int_{\mathbb{T}} [u^\Delta(w \circ \nu)](t) \Delta t \\
&= \int_{\mathbb{T}} [u^\sigma(w \circ \nu)^\Delta + u^\Delta(w \circ \nu)](t) \Delta t \\
&= \int_{\mathbb{T}} [u(w \circ \nu)]^\Delta(t) \Delta t \\
&= u(b)w(\nu(b)) - u(a)w(\nu(a)).
\end{aligned}$$

Now the statement of the theorem follows. ■

As usual, if operators A and B on $\tilde{\mathbb{T}}$ and \mathbb{T} , respectively, satisfy

$$\langle u, Aw \rangle_{\mathbb{T}} = \langle Bu, w \rangle_{\tilde{\mathbb{T}}}, \quad \text{for all } u \in \mathbb{T}, \quad w \in \tilde{\mathbb{T}},$$

then we call B the *adjoint* of A (we write $B^* = A$). We obtain the following consequence of Theorem 4.1.

COROLLARY 4.1. *For Dirichlet boundary conditions, the divergence and the gradient are negative adjoints of each other, i.e., if $u(a) = u(b) = 0$, then $\text{grad}^* = -\text{div}$.*

Another result is obtained by putting $w = \text{grad } u$ in Theorem 4.1.

COROLLARY 4.2. *If u is differentiable on \mathbb{T} , then we have*

$$\langle u, \text{div grad } u \rangle_{\mathbb{T}} + \langle \text{grad } u, \text{grad } u \rangle_{\tilde{\mathbb{T}}} = u(b) \text{grad } u(\nu(b)) - u(a) \text{grad } u(\nu(a)).$$

As usual, if an operator A satisfies

$$\langle u, Au \rangle \leq 0, \quad \text{for all } u \in \mathbb{T},$$

then we call A *negative semidefinite* (we write $A \leq 0$). Note that

$$\langle \text{grad } u, \text{grad } u \rangle_{\tilde{\mathbb{T}}} = \int_{\mathbb{T}} (\text{grad } u(t))^2 \tilde{\Delta} t \geq 0.$$

Hence, Corollary 4.2 says that, e.g., for Dirichlet boundary conditions the operator div grad (the so-called *Laplacian*) is *negative semidefinite*, i.e., if $u(a) = u(b) = 0$, then $\text{div grad} \leq 0$.

5. CONCLUSIONS

We have shown a strong connection between mimetic differential operators, which are discrete, and their analog continuous operators via the calculus of time scales (or measure chains). We introduced the divergence and gradient operator for functions defined on a measure chain. We then showed in the one-dimensional case, with Dirichlet boundary conditions, that the divergence and the gradient are negative adjoints of each other and that the divergence of the gradient (or the Laplacian) is negative semidefinite. Future work contemplates the generalization of these properties to higher dimensions.

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