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High Order Mimetic Differences and Applications *

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Abstract

Mimetic methods construct discrete numerical schemes based on discrete analogs of spatial differential vector calculus operators like divergence, gradient, curl, Laplacian, etc. They mimic solution symmetries, conservation laws, vector calculus identities, and other important properties of continuum partial differential equations models. The original versions of these methods were restricted to be of low-order of accuracy. High-order mimetic operators were later introduced, first by Castillo and Grone at San Diego State University, via the introduction of convenient inner product weights to enforce a discrete high-order extended Gauss divergence theorem, and later by a collaboration of Los Alamos National Laboratory and a group of researchers at Milano-Pavia. This review focuses on the developments of high-order mimetic differences by Castillo and his group at San Diego and the utilization of these techniques to different applications. In addition, when appropriate, it exhibits similarities and differences between the two methodologies.

1 Introduction

This paper is about the high-order mimetic differences (MD) numerical method of Castillo and Grone [1] and its more accurate and compact version of Corbino and Castillo [2], their history and applications to science and engineering mathematical models. MD is a classical mimetic methodology, in the sense that it constructs discrete analogs of operators in such a way that they enforce high-order accuracy of the extended Gauss divergence theorem, a generalization of the integration by parts (IBP) formula.

This document also contain, when relevant, MD likeness and distinction with respect to the Mimetic Finite Difference (MFD) method [3], an evolutionary hybrid between classic mimetic methods, and a fully mimetic approach. For fully mimetic style, we understand a technique that constructs a discrete version of either continuum vector [4], tensor [5],

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or exterior [6, 7] calculi, so it resembles differential geometry, via the utilization of some algebraic topology tools [8].

Furthermore, we describe the development and the utilization of the Mimetic Operator Library Enhanced (MOLE) [9], an open source library written by J. Corbino, to facilitate the usage of MD operators in the numerical solution of systems of Partial Differential Equations (PDEs), in one-dimension (1D), two-dimensions (2D) and three-dimensions (3D).

Section 2, gives some history of mimetic methods, and when appropriate, it compares MD with MFD. Section 3, introduces MD. Section 4, display some MD current developments. Section 5, review some of the applications solved with MD. Section 6, include some conclusions of this paper.

2 History of mimetic methods

Traditional discretization techniques for the numerical solution of PDE initial and/or boundary value problems began with finite difference methods [10, 11, 12, 13]. Flux conservation considerations across the boundary of computational cells derived in the formulation of the finite volume method [14]. Discretization of Sobolev spaces, the more natural functional spaces that are considered the widest extensions of smooth functions, appear in the variational formulations of PDE theory [15], where solutions are understood in the weak sense rather than in the classical smooth sense, unfold the finite element method [16]. One can notice that the incremental progress in the genesis of PDE numerical schemes gradually imposes more requirements on the methods been evolved for approximately solving PDEs. One of the latest examples in the improvement of these approaches has been the introduction of spectral methods [17]. In this category of methods one can find (RBF) [18], and Summation By Parts (SBP) [19] methods, where the utilization of Fourier series expansions, in the quest for finding a high-order accurate approximate solution, tend to incorporate additional terms in the PDE discretization, in order to satisfy some physical properties of its continuous PDE.

Mimetic methods can be seen as one of the latest stages in this emergence process. They are based on discrete analogs of spatial differential operators such as gradient, divergence, curl, and Laplacian. Mimetic operators aim to satisfy, in the discrete sense, properties that the continuum operators do. Historically, this has been understood in two manners, one where the characteristics to be mimicked follow from enforcing certain integral theorems, and another where what is pursued is the construction of a discrete calculus that replicates the continuum properties of vector, tensor, exterior, calculi. For example, in the first avenue, mimetic methods are expected to mimic solution symmetries, conservation laws, vector calculus identities, and other important properties of continuum PDE mathematical models as a consequence of imitating one of the vector calculus fundamental theorems [20], or Green's identities [15] derived from the different differentiation of product rules [21, 1, 2]. On the second case, mimetic methods are called fully mimetic and are based on constructing

a discrete calculus that mimics properties of the corresponding continuum one. In this last category one can find fully mimetic methods that elaborate a discrete vector calculus [4], tensor calculus [3, 5], exterior calculus [7, 6, 8], and others based on algebraic topology [22, 23].

Even though, originally the technique was not called that way, early work in mimetic methods was developed by A.A. Samarskii at Moscow State University during the middle of the twentieth century [3, 24, 25] and independently at Los Alamos National Lab [26]. Because of its implementation simplicity, mimetic methods were built initially utilizing finite differences. These techniques were originally translated into English as the support-operator method (SOM) [21]. These approaches have been utilized in a plethora of applications since then by a team of researchers mainly at Los Alamos National Laboratory (LANL) [3, 21].

It turned out that SOM as well as any other classical mimetic method were low-order accurate. Aware of this SOM limitation, in 2003 Castillo and Grone [1] introduced the high-order MD operators that are uniformly accurate on staggered grids, with inner products given by non-canonical positive diagonal weights and whose gradient, divergence and curl operators are given by parameterized families of operators, with the number of parameters varying accordingly to the degree of accuracy of the corresponding operators. MD was historically the first mimetic approach that attains high-order accurate operators and it is until today, the unique mimetic modus operandi to achieve uniform high-order accuracy over the whole computational domain, interior and boundary included.

Such mimetic difference operators were constructed specifically to satisfy high-order discrete analogs of the fundamental theorem of calculus and the IBP formula [1, 27]. Later, with the introduction of high-order mimetic interpolation operators [28], it was possible to show that these operators satisfy the extended Gauss divergence theorem as well as fundamental vector calculus identities [29]. These operators are built on a staggered mesh. The discrete mimetic difference operators, divergence and gradient, are constructed independently of each other as is the case of the divergence and gradient in vector calculus.

More recently, in 2019, Corbino-Castillo [2] found a unique (without parameters) similar high-order mimetic difference operators satisfying the same properties of the Castillo-Grone operators which can be implemented in a compact way so they use a short stencil and are local not as compact finite differences which are global.

In addition, MOLE (mimetic operator library enhanced), an open source library for the Corbino-Castillo operators, was developed at the time by J. Corbino [9]. This software library, written in MATLAB/Octave and C++, is not a black-box and it provides functionality for researchers that want to utilize MD operators for solving numerically PDEs. Dozens of examples, and a basic user guide are readily available from the MOLE GitHub repository [9]. The library has been successfully used by a few research groups around the globe and by San Diego State University (SDSU) students in class and research projects. MOLE provides developers the ability to rapidly model numerical solutions to complex relations in field theory by expressing, in code, the connection in familiar differential form.

The ability to codify solutions in a canonical form, without loss of accuracy, reduces time and cost for rapid prototyping of highly accurate and computationally efficient computer codes to solve complex problems.

There are several features that make MD a very singular approach when compared to other mimetic techniques. Among those,

- It does not utilize explicitly a primal and a dual grid.
- It does not work with dual spaces.
- The gradient and divergence operators are constructed independently of each other. In other classical methods, a primary operator is defined and then by utilizing Green's identities, dual operators are derived. Fully mimetic operators utilize double exact sequences of skew-symmetric forms and tensors of different orders to define gradient, curl and divergence operators. This is because, what it is enforced in MD is the Schwarz' theorem of mixed derivatives.
- It does not use integrals or averages projections over a certain regions to discretize the continuum spaces, and hence it uses point-wise versions of the first-order differential operators instead of their integral versions.
- It achieves uniform high-order of accuracy. Other approaches loss accuracy on the boundary.
- It uses data from nearest cell neighbors to attain high-order accuracy, instead of increasing degrees of freedom in an element-wise form. Because of this, the resulting system of equations are sparser than those of other mimetic methodologies.
- Corbino-Castillo operators are implemented in a local compact way, instead of the usual global way. Castillo-Grone operators can also be implemented in a similar way.
- High-order mimetic interpolation operators are constructed explicitly for moving data throughout the staggered grid [28]. The importance of interpolation operators shows up disguised in other approaches as an implicit part of reconstruction operators.
- Explicit high-order quadrature weight operators that enforce a high-order discrete analog of the extended Gauss divergence theorem are fabricated.
- Its implementation is simple since it works with non-uniform curvilinear structured Cartesian grids.

3 Mimetic differences

Due to the several singular features that make MD a unique method, in this section, we review how the characterization of the different operators have evolved in time.

3.1 The Castillo-Grone approach

Originally, the 2003 Castillo-Grone MD operators were derived such a way that they comply with the following definition of being mimetic:

1. To find higher-order approximations of the divergence and gradient that satisfy a discrete analogue of the divergence theorem:

$$\int_U \vec{v} \cdot \nabla f \, dU + \int_U f \nabla \cdot \vec{v} \, dU = \int_{\partial U} f \vec{v} \cdot \vec{n} \, dS. \quad (1)$$

2. Local conservation ((1) applied to $f \equiv 1$ and U a single cell).
3. Global conservation ((1) applied to $f \equiv 1$ and U full region).

In 1D, for example in $[0, 1]$, (1) becomes the IBP formula, which for $f \equiv 1$ is the Fundamental Theorem of Calculus (FTC).

In 2D and 3D, gradient operators applied on scalar fields and return vector fields and divergence operators apply on vectors fields and return scalar fields. This is extended to 1D. In 1D, MD utilizes a staggered grid composed of centers or boundaries \mathcal{C} (where discrete versions of scalar fields are defined), and nodes or boundaries \mathcal{N} (where discrete versions of vector fields are defined), both sets having different cardinalities. Therefore, the discrete analog of the gradient operator is a map $G : \mathcal{C} \rightarrow \mathcal{N}$, and the discrete analog of the divergence operator is a map $D : \mathcal{N} \rightarrow \mathcal{C}$. Physical considerations lead to set D to zero on the boundaries [27]. Observe that both discrete representations are non-square matrices. The discrete analogs of the curl operator C are defined by utilizing D . The discrete analogs of first-order vector calculus differential operators can be built to be high-order accurate. Typical orders of accuracy are $k = 2, 4, 6, 8$. The discrete analogs of the 2D and 3D corresponding operators are obtained via Kronecker products.

Mimicking in 1D the property that the divergence of a constant vector field is zero, demands that the row sums of D must be zero. The FTC imposes that D column sums match $(-1, 0, \dots, 0, 1)$. Symmetry with respect to the boundary points requires that $P_N D P_{N+1} = -D$, where P_n the $n \times n$ permutation matrix such $P_{ij} = \delta_{i, n+1-j}$. It is also desired for D to be sparse and banded with bandwidth b . Furthermore, the stencil for interior nodes should be similar and hence interior rows should exhibit a Toeplitz-type structure and D have to be exact for polynomials of order up to k but not $k + 1$. At the boundary the divergence is set to zero. To get k -th order accuracy at the $k - 1$ nearest centers, the stencil for D uses $\frac{3k}{2}$ nearest nodal neighbors (including the boundary point). It is also required a uniform order of accuracy at the boundary. The stencil near the boundary is represented by $A_k \in \mathbb{R}^{k \times \frac{3k}{2}}$. It is required that $N \geq 3k - 1$, where N is the number of

cells. For Castillo-Grone, the form of D is

$$D = \begin{bmatrix} A_k & 0 & 0 \\ S_k & & \\ & S_k & \\ 0 & 0 & -P_k A_k P_k \end{bmatrix}. \quad (2)$$

Therefore, a summary of the mimetic divergence D properties are:

- D is a $N \times (N + 1)$ matrix.
- D has zero row sum.
- D has column sums $(-1, 0, \dots, 0, 1)$.
- D is banded.
- D has a Toeplitz-type structure away from the boundary grid points.
- D is center-skew-symmetric.
- D is of the form (2).

The gradient operator G should hold similar properties.

The k -th order of accuracy conditions for points near the boundary are expressed in terms of a series of Vandermonde matrices. It turns out that there exist parametrized families of stencils that satisfy the boundary requirements. For example, for order $k = 4$, a 3-parameter family of solutions exist. It is possible to choose the parameter values such that the boundary stencils resemble as much as possible the inner stencils.

Moreover, the IBP formula should hold. It requires that the discrete analog of (1) for $U = [0, 1]$,

$$\langle Dv, f \rangle + \langle v, Gf \rangle = v_N f_N - v_0 f_0,$$

where the angular brackets mean that the integrals are approximated utilizing a classic quadrature, and should hold with high-order accuracy. However, this is not possible unless special weighted inner products are introduced, meaning P and Q , and

$$\langle Dv, f \rangle_Q + \langle v, Gf \rangle_P = v_N f_N - v_0 f_0. \quad (3)$$

3.2 Non-uniform structured meshes

In 2009, E.D. Batista et al. [30], extended MD for working on non-uniform structured Cartesian grids. Discrete analogs of first-order differential operators divergence D and gradient G , which for uniform meshes are $D = \frac{1}{h} D_u$ and $G = \frac{1}{h} G_u$, where h is the cell size, with the sub-indices u stand for uniform, and D_u, G_u mean the corresponding operators of uniform grid of size 1. For the non-uniform grid $x = [x_0, x_1, \dots, x_{N_1}, x_N]$, the non-uniform operators D_n, G_n become $D_n = \text{diag}\{(D_u x)^{-1}\} D_u$, $G_n = \text{diag}\{(G_u x)^{-1}\} G_u$.

Hence,

$$\begin{bmatrix} s_1 & s_2 & s_3 & s_4 \end{bmatrix} \begin{bmatrix} 1 & -\frac{3}{2} & \frac{3^2}{2^2} & -\frac{3^3}{2^3} & \frac{3^4}{2^4} \\ 1 & -\frac{1}{2} & \frac{1}{2^2} & -\frac{1}{2^3} & \frac{1}{2^4} \\ 1 & \frac{1}{2} & \frac{1}{2^2} & \frac{1}{2^3} & \frac{1}{2^4} \\ 1 & \frac{3}{2} & \frac{3^2}{2^2} & \frac{3^3}{2^3} & \frac{3^4}{2^4} \end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{h} & 0 & 0 & 0 \end{bmatrix}$$

It turns out that the unique solution for the weights is $(s_1, s_2, s_3, s_4) = (\frac{1}{24h}, -\frac{9}{8h}, \frac{9}{8h}, -\frac{1}{24h})$.

Similarly, the fourth-order local truncation error for points at or near the boundary. For example, the divergence at the boundary x_0 is zero by definition. Then one focuses on calculating $f'(x_{h/2})$ is calculated in terms of f at $x_0, x_h, x_{2h}, x_{3h}, x_{4h}, x_{5h}$. In that case, for finding the weights one needs to construct the corresponding Vandermonde matrix and to solve

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -\frac{1}{2} & \frac{1}{2} & \frac{3}{2} & \frac{5}{2} & \frac{7}{2} & \frac{9}{2} \\ (-\frac{1}{2})^2 & (\frac{1}{2})^2 & (\frac{3}{2})^2 & (\frac{5}{2})^2 & (\frac{7}{2})^2 & (\frac{9}{2})^2 \\ (-\frac{1}{2})^3 & (\frac{1}{2})^3 & (\frac{3}{2})^3 & (\frac{5}{2})^3 & (\frac{7}{2})^3 & (\frac{9}{2})^3 \\ (-\frac{1}{2})^4 & (\frac{1}{2})^4 & (\frac{3}{2})^4 & (\frac{5}{2})^4 & (\frac{7}{2})^4 & (\frac{9}{2})^4 \end{bmatrix} \begin{bmatrix} a_{11} \\ a_{12} \\ a_{13} \\ a_{14} \\ a_{15} \\ a_{16} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{h} \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

whose solution is a one-dimensional affine linear space given by

$$[a_{11}, a_{12}, a_{13}, a_{14}, a_{15}, a_{16}] = \frac{1}{h} \left[-\frac{11}{27}, \frac{17}{24}, \frac{3}{8}, -\frac{5}{24}, \frac{1}{24} \right] + \frac{\alpha}{h} [-1, 5, -10, 10, -5, 1]. \quad (4)$$

Usually parameter α is chosen so one can replicate the stencil for the interior points, when possible.

3.4 The Simplex approach for weights

If in (1), for N cells, one assumes the constant discrete scalar field $F = \mathbf{1} \in \mathbb{R}^{N+2}$, then it implies

$$h \langle DV, \mathbf{1} \rangle_Q = V_N - V_0,$$

and, since $\langle DV, \mathbf{1} \rangle_Q = \langle QDV, \mathbf{1} \rangle = \langle V, D^T Q \mathbf{1} \rangle = V^T D^T Q \mathbf{1}$, then

$$h V^T D^T Q \mathbf{1} = V^T (-1, 0, \dots, 0, 1)^T,$$

or equivalently, if $b_{N+1} = (-1, 0, \dots, 0, 1) \in \mathbb{R}^{N+1}$ then

$$h D^T Q \mathbf{1} = b_{N+1}^T, \quad (5)$$

which is utilized to find the unique weight matrix Q .

In 2015, Sanchez et al. [32, 33], noticed that weight equations similar to (5) have a unique solution q , and that for order of accuracy $k \geq 8$, some q_i are negative.

From the fact that solving (5) is equivalent to solving the linear programming problem

$$\begin{aligned} z &= \min q_1 + \dots + q_{N+1} \\ h D^T Q \mathbf{1} &= b_{N+1}^T, \end{aligned}$$

then, the authors proposed a linear programming problem for the parametrized Kernel of the discrete divergence operator to demonstrate that one can always find diagonal positive definite Q . Similarly for P .

In addition, the Mimetic Methods Toolkit (MTK), an object-oriented API for implementing Castillo-Grone MD was implemented [34]. MTK worked with full matrices.

3.5 Extensions to nonlinear PDEs on complex geometries

In 2019, A. Boada introduced a methodology for solving anisotropic Laplacian [35] with rough coefficients via smart interpolations [36]. In addition, with the utilization of invertible domain maps, he was able to solve PDEs defined over curvilinear structured grids. In his technique, there are two versions of both map Jacobian and inverse map Jacobian based on how first-order partial derivatives are computed via the discrete analog of the divergence or gradient operators. Moreover, utilizing the open-source library Overture [37], he demonstrate the capability of MD for working with overlapping grids. Furthermore, he also demonstrated the ability of solving some nonlinear PDEs with MD operators.

3.6 The Corbino-Castillo approach

In 2020, J. Corbino et al. [2], following a finite difference approach, introduced the Corbino-Castillo MD method. This MD version achieves higher-order weight quadratures than the corresponding Castillo-Grone ones, and its operators are implemented in a compact way, which is local, instead of the usual way compact finite differences are global. The main difference between the two mechanisms is that, the matrix A in the derivation of the the discrete analogs of the divergence and gradient operators (2) are smaller, i.e., $A \in \mathbb{R}^{k \times (k+1)}$. Notice that instead of having $\frac{3k}{2}$ columns, it has only $k + 1$. This new size of stencil triggers that the discrete analogs of D and G do not have free parameters and in this way the families reduce to only one member.

This new approach leverages on all the previous extensions of the Castillo-Grone method. Moreover, MOLE [9] was implemented. It allows to work with sparse matrices. MOLE substituted MTK because of its better accuracy, memory efficiency and speed when solving numerically PDEs.

4 Posterior developments

Several recent development have improved MD not only from the theoretical point of view but also from practical issues that raise when trying to use high-order operators for numerically solving PDEs.

4.1 Computing operator coefficients exactly

The construction of MD high-order divergence and gradient operators is facilitated by inverting several Vandermonde matrix (with appropriate rational generators $c = (c_1, \dots, c_p)$), which for high-order operators might have large condition numbers. Software packages may introduce numerical errors when computing them. It can be proven that discrete analogs of the divergence and gradient require only the second row of the inverse of a Vandermonde matrix. In [38] one can find exact simple formulas for those coefficients. Exact divergence and gradient coefficients can be computed this way. These formulas are utilized in [29]. In particular, the entry (i, j) , $1 \leq i, j \leq p$, of its inverse \mathbb{V}^{-1} is given by:

$$\left\{ \begin{array}{ll} (\mathbb{V}^{-1})_{i,j} = \frac{(-1)^{i+j} S_{p-i,j}}{\prod_{l < q} (c_q - c_l)}, & l = j, \text{ or } q = j, \\ S_{q,j} = S_q(c_1, \dots, c_{j-1}, c_{j+1}, \dots, c_p), & 1 \leq q \leq p-1, 1 \leq j \leq p, \\ S_q = S_q(c_1, \dots, c_p) = \sum_{1 \leq i_1 < \dots < i_q \leq p} c_{i_1} \dots c_{i_q}, & 1 \leq q \leq p, \\ S_0 = S_0(c_1, \dots, c_p) = 1, & \\ S_q = 0, & q \notin \{0, 1, \dots, p\}. \end{array} \right.$$

4.2 High-order Interpolation operators

Divergence and gradient operators live in different grid points and sometimes it is not possible to compute products of scalar and vector fields. The need for high-order interpolation appears vivid for example when trying to verify with high-order accuracy the extended version of the Gauss divergence theorem, or when attempting to corroborate the discrete analog of the divergence of the product of a scalar and a vector field.

Utilizing Kronecker products [39], it was possible to introduce MD high-order interpolation operators in 2D and 3D. They are based on 1D interpolation operators, which utilize the methodology presented in [38] for computing the coefficients in the first row of the inverse of a Vandermonde matrix.

Interpolation operators from centers to nodes in d -dimensions have the following struc-

4.4 Vector calculus identities

It is expected that discrete analog MD operators should verify vector calculus identities.

Castillo-Grone and Corbino-Castillo MD approaches satisfy, by construction, a discrete analog of the IBP formula, and that is central in the formulation of the methods. This property and their consequences are essential for deriving weights Q, P .

Nevertheless, this explicit requirement imposes an integral condition that implicitly facilitates the demonstration of high-order discrete analogs of the integral version of vector calculus identities instead of their differential form.

This is why [1] introduced matrices P and Q that induce inner products associated to the gradient and divergence mimetic operators, respectively. Therefore, discrete analogs of vector calculus identities should be understood in the integral sense. However, it is possible to prove second-order versions of some of the differential form vector calculus identities.

Of special interest is the gradient of a product identity,

$$\nabla(fg) = f \nabla g + g \nabla f.$$

which no other not fully mimetic method is able to demonstrate [29].

Other important identities are the divergence of a product

$$\nabla \cdot (f \vec{v}) = \nabla f \cdot \vec{v} + f \nabla \cdot \vec{v},$$

and the Laplacian of a product

$$\Delta(fg) = f \Delta g + 2 \nabla f \cdot \nabla g + g \Delta f.$$

4.5 Energy conservation

It is relatively simple to show energy conservation with MD schemes.

4.5.1 For the 1D advection equation

Consider the following one-dimensional advection PDE

$$\begin{aligned} u_t + u_x &= 0, & x \in (-1, 1), & t > 0, \\ u(-1, t) &= g(t), & t > 0, \\ u(x, 0) &= u_0(x), \end{aligned} \tag{6}$$

with a condition on the left boundary, and an initial condition.

By multiplying (6) by u and integrating over the spatial domain, after a time integration from 0 to T , one gets

$$\left(\int_{-1}^1 (u^2(x, T) - u^2(x, 0)) dx \right) + \int_0^T \int_{-1}^1 \nabla \cdot (u^2) dx dt = 0. \tag{7}$$

Now, one writes the mimetic discrete analog of (7). Observe that any discretization of the first integral $\int_{-1}^1 u^2(x, t) dx$ will generate the energy difference at times $t = T$ and $t = 0$.

If $U(x, t)$ is a mimetic numerical approximation of $u(x, t)$, for on the cell centers of the staggered grid $x \in \{-1 = x_0, x_{\frac{1}{2}}, \dots, x_{N-\frac{1}{2}}, x_N = 1\}$, with $h = \frac{1}{N}$ and $x_{j-\frac{1}{2}} = -1 + (j - \frac{1}{2})h$, $j = 1, \dots, N$, then the mimetic discrete analog of the FTC states that

$$\begin{aligned} \mathbf{1} QD(I_D U^2) &= (-1, 0, \dots, 0, 1) \cdot (U^2(x_0, t), U^2(x_1, t), \dots, U^2(x_{N-1}, t), U^2(x_N, t))^T \\ &= -U^2(-1, t) + U^2(1, t), \end{aligned} \quad (8)$$

and hence using the boundary condition, (7) becomes,

$$E(T) + \frac{1}{h} \int_0^T U^2(1, t) dt = E(0) + \frac{1}{h} \int_0^T g^2(t) dt,$$

i.e., the energy at T plus the energy lost at the right boundary matches the initial energy plus the energy gained at the left boundary.

4.5.2 For the 3D advection equation

Consider the 3D advection PDE on $V = [-1, 1]^3$, with constant velocity $v = (v_1, v_2, v_3)^t$,

$$\begin{aligned} u_t + \nabla \cdot (uv) &= 0, & (x, y, z) \in V, \quad t > 0, \\ u(-1, y, z, t) &= g_1(y, z, t), & (x, y, z) \in \{-1\} \times (-1, 1) \times (-1, 1), \quad t > 0, \\ u(x, -1, z, t) &= g_2(x, z, t), & (x, y, z) \in (-1, 1) \times \{-1\} \times (-1, 1), \quad t > 0, \\ u(x, y, -1, t) &= g_3(x, y, t), & (x, y, z) \in (-1, 1) \times (-1, 1) \times \{-1\}, \quad t > 0, \\ u(x, y, z, 0) &= u_0(x, y, z), & (x, y, z) \in V, \end{aligned} \quad (9)$$

where g_1, g_2, g_3, u_0 , are smooth enough functions, such there is enough differentiability among their values on the common boundaries. By multiplying (9) by u and integrating over the spatial domain, and after a time integration from 0 to T , one gets

$$\int_V (u^2(x, y, z, T) - u^2(x, y, z, 0)) dx + \int_0^T \int_V \nabla \cdot (u^2 \vec{v}) dV dt = 0. \quad (10)$$

Similarly, as in the 1D case, the first term will become $E(T) - E(0)$, where $E(t)$ is the energy at t . The mimetic approximation of order k for $\int_V \mathbf{1} \nabla \cdot (u^2 \vec{v}) dV$, is given by

$$\langle D_{xyz}^k(\vec{\mathcal{V}} \mathcal{I}_D^k(U^2)), \mathbf{1} \rangle_{\mathcal{Q}^k} = \text{vec}_L(\vec{\mathcal{V}} \mathcal{I}_D^k(U^2))^T \mathcal{Q}^k (D_{xyz}^k)^T \text{vec}_L(\mathbf{1}), \quad (11)$$

where $\mathbf{1}$ is the constant one discrete scalar field, $\vec{\mathcal{V}}$ is the discrete version of constant vector field \vec{v} , and vec_L is the vectorization operator following the lexicographic ordering.

As indicated in [40], a direct computation of $\mathcal{Q}^k(D_{xyz}^k)^T \text{vec}_L(\mathbf{1})$ gives

$$\mathcal{Q}^k(D_{xyz}^k)^T \text{vec}_L(\mathbf{1}) = \begin{bmatrix} (\hat{I}_o^T \otimes \hat{I}_n^T \otimes Q_{m+2}^k D_x^{kT}) \text{vec}_L(\mathbf{1}) \\ (\hat{I}_o^T \otimes Q_{n+2}^k D_y^{kT} \otimes \hat{I}_m^T) \text{vec}_L(\mathbf{1}) \\ (Q_{o+2}^k D_z^{kT} \otimes \hat{I}_n^T \otimes \hat{I}_m^T) \text{vec}_L(\mathbf{1}) \end{bmatrix}. \quad (12)$$

Since $(B^T \otimes A) \text{vec}_L(X) = \text{vec}_L(AXB^T)$, the first row of (12) becomes

$$[Q_{m+2}^k D_x^{kT} \mathbf{1}_{m+2, (n+2)(o+2)}] (\hat{I}_o \otimes \hat{I}_n) = [-1, 0, \dots, 0, 1]_m^T [1, \dots, 1]_{no}.$$

Similarly, the other two rows. One can observe the resemblance to (8). This suggests already the conservation of energy achieved in the 1D case.

Additional discrete analogs for energy preservation of conservation laws is currently being studied.

4.6 Consistency, stability, and convergence

In [40], it has been shown that the MD semi-discrete analog of equation

$$u_t = -\nabla \cdot (u\vec{v}),$$

could be written as

$$U_t = KU,$$

for $K = K_D$ or $K = K_G$, where

$$K_D = - \left[D_{xyz}^k \begin{pmatrix} \text{diag}(V_1) & & \\ & \text{diag}(V_2) & \\ & & \text{diag}(V_3) \end{pmatrix} \mathcal{I}_D^k \right].$$

and

$$K_G = -\mathcal{I}_G^k \left[\begin{pmatrix} \text{diag}(V_1) & & \\ & \text{diag}(V_2) & \\ & & \text{diag}(V_3) \end{pmatrix} G_{xyz}^k \right].$$

If one utilizes the second-order time discretization, referred to as the formulation of fifth-order leap frog filtered scheme in [41],

$$\psi^{s+1} - \bar{\psi}^{s-1} = 2\Delta t F(\psi^s),$$

where

$$\bar{\psi}^{s-1} = \psi^{s-1} + \gamma_6 (\bar{\psi}^{s-4} - 5\bar{\psi}^{s-3} + 10\bar{\psi}^{s-2} - 10\bar{\psi}^{s-1} + 5\psi^s - \psi^{s+1}),$$

one can prove consistency, stability and convergence of the resultant mimetic scheme by rewriting the time discretization, for $\bar{\gamma}_6 = (1 + 11\gamma_6)^{-1}$, as

$$\begin{aligned}\bar{\psi}^{s-1} &= \bar{\gamma}_6(\tilde{\psi}^{s-1} - 2\gamma_6\Delta t F(\psi^s)), \\ \psi^{s+1} &= \bar{\gamma}_6(\tilde{\psi}^{s-1} + 2(1 + 10\gamma_6)\Delta t F(\psi^s)), \\ \tilde{\psi}^s &= \psi^s + \gamma_6(\bar{\psi}^{s-3} - 5\bar{\psi}^{s-2} + 10\bar{\psi}^{s-1} + 5\psi^{s+1}),\end{aligned}$$

which is parametrized by four quantities which get updated following the iterative algorithm that overwrites

$$(\bar{\psi}^{s-3}, \bar{\psi}^{s-2}, \tilde{\psi}^{s-1}, \psi^s) \quad \text{by} \quad (\bar{\psi}^{s-2}, \bar{\psi}^{s-1}, \tilde{\psi}^s, \psi^{s+1}).$$

4.7 Quadratures

This study was inspired by the resemblance of the coefficients of the mimetic quadratures with those of Newton-Cotes'. Actually, the second-order is exactly the 3/8, 9/8 Newton-Cotes quadratures, as previously it was noticed by [42]. The results of [43] and [44] demonstrated that mimetic quadrature weight coefficients are a possible alternative for numerical integration. This ansatz is extended for fourth and sixth-order of accuracy weight operators. These quadratures satisfy the divergence theorem [45].

4.8 Other developments

There exist several current MD developments. Among them:

- Stability analysis of the Castillo-Grone MD [46, 47].
- MD discrete analog curl operator is defined in terms of the discrete analog of the divergence. A more independent curl representation is being pursued.
- Even though, utilizing high-order interpolation operators helps to perform the different products between scalar and vector fields, frequency in their usage could degrade the higher-order accuracy targeted by the mimetic schemes. One aims at defining scalar and vector fields everywhere removing most of the need for interpolations.
- Extending MD to problems with interfaces.
- Embedding and/or extending MD to become a fully mimetic technique.
- Extending MD to adaptive mesh refinement, to focus in parts of the domain that need more detail of the solution.
- Reformulating how to handle boundary conditions in general.
- Assimilating the previous advancements into the MOLE.

5 Applications

PDEs have been used to model phenomena over decades in many fields that have a great societal impact such as medicine, geophysics, climate change, electrodynamics, finance, economics, weather forecasting, wireless communication, transportation, advancements in computation, reorganization of food production chains, and quantum mechanics phenomena, which are fundamental for the understanding of complex systems. Explicit, closed-form solutions to many PDEs are unattainable to obtain analytically, rendering numerical approximations the only viable alternative.

MD methods are based on developing discrete analogs for tensor calculus identities of divergence and gradient, which are used to accurately discretize continuum models for a wide range of physical processes [48]. These discrete operators preserve the properties of their continuum ones, and thus allow for the discretization of PDEs to mimic critical properties such as conservation laws and symmetries. The models of boundary value problems solved using the mimetic operators often produce results with more meaningful physical interpretation [49].

MD discretization schemes on non-uniform meshes were initially studied by [50, 30]. The discretizations for the first derivative were based on the projections of the vector calculus identities of divergence and gradient operators.

MD schemes have been successfully implemented to solve PDEs in a variety of applications such as the anisotropic elliptic equation [35], unsaturated flows using Richards' equation [51], modeling geologic storage for carbon dioxide [52], image processing [53], rupture propagation in earthquakes [54] and acoustic wave propagation [55, 56]. In addition, they have been used to solve the Poisson equation on curvilinear meshes [57] and on non-uniform meshes [30]. Moreover, MD has been implemented on non-trivial problems (i.e., PDEs with rough coefficients, irregular domains, overlapping grids, non-linearities and combinations thereof) [36].

To date, MOLE has already been employed in modeling solutions in seismic imaging, rupture propagation, low dispersive Rayleigh waves, wave propagation in geophysics, glaucoma detection, restorative medicine, ocean-atmosphere modeling in weather forecasting, and unsaturated flow in fluid mechanics. Some examples in these research/application areas are: seismic imaging [58, 59], rupture propagation [60], low dispersive Rayleigh waves [61], wave propagation [55] in Geophysics; glaucoma detection [62] and restoration [63] in Medicine; ocean-atmosphere modeling [64] in Weather Forecast, and unsaturated flow [65] in Fluid Mechanics.

It is worth to mention that MD has been recognized as a fast, accurate and successful method in the are of geophysics [66, 67], when compared to other numerical methods [58].

6 Conclusions

This is a paper about high-order mimetic differences, identified by MD in this document. We began introducing mimetic methods in general, and gave the characteristics that make MD successful and singular among other mimetic approaches. We have discussed the main milestones during the MD evolution, since its inception twenty years ago of the Castillo-Grone methodology. Amid the particular challenges that guided the historical progression of MD, one finds initially a finite difference formulation of this technique to obtain discrete analogs of the divergence and gradient operators. Later on, the exigency of constructing diagonal positive definite weights for the inner products used for approximating integrals and that can achieve high-order accuracy of the discrete analog of the integration by parts formula, triggered the linear programming perspective based on the linear constraints imposed on these weight operators by the presence of the discrete analogs of the Fundamental Theorem of Calculus. The need of working with non-uniform grids, curvilinear structured meshes, and dealing with PDEs that contain rough coefficients, anisotropic Laplacian operator, overlapping grids, and non-linearities, generated several extensions of MD to deal with those issues, as well as the development of the Mimetic Toolkit Library. The Corbino-Castillo approach surged as an attempt to reformulate MD to have local compact stencils, reduce the operators bandwidth, and remove the free parameters of its machinery. As a result of this conception, the open-source Mimetic Operators Library Enhanced, that allows working with sparse matrices, was implemented. In some of the mentioned stages of MD advancement, we have provided some hints about how MD addresses those matters.

This review also show more recent theoretical and practical MD improvements, both for Corbino-Castillo and Castillo-Grone variants. These include ways of computing the operator coefficients exactly; the introduction of several high-order interpolation operators to move different quantities of the staggered grid without losing precision; the confirmation that discrete analogs of vector calculus identities hold via mathematical proofs; the establishment of energy conservation for different partial differential equations; the validation of consistency, stability, and convergence of mimetic schemes when utilizing time discretization formulas with several stages; the extension of MD weight operators as high-order quadratures; and finally we point out a few avenues of current MD exploration such problems with interfaces, new curl and boundary condition operators, as well as, the creation of a fully staggered approach and a fully mimetic flavour of it. The new MD features are being added to the Mimetic Operators Library Enhanced, as soon as, the corresponding source codes pass some intensive testing.

It is in our plans to consolidate the Castillo-Grone operators to this latter library, to offer versions of it in other programming languages, to expand the community of its users worldwide, to promote MD, and exhibit its capacities for solving systems of partial differential equations and to blend with other numerical methods.

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