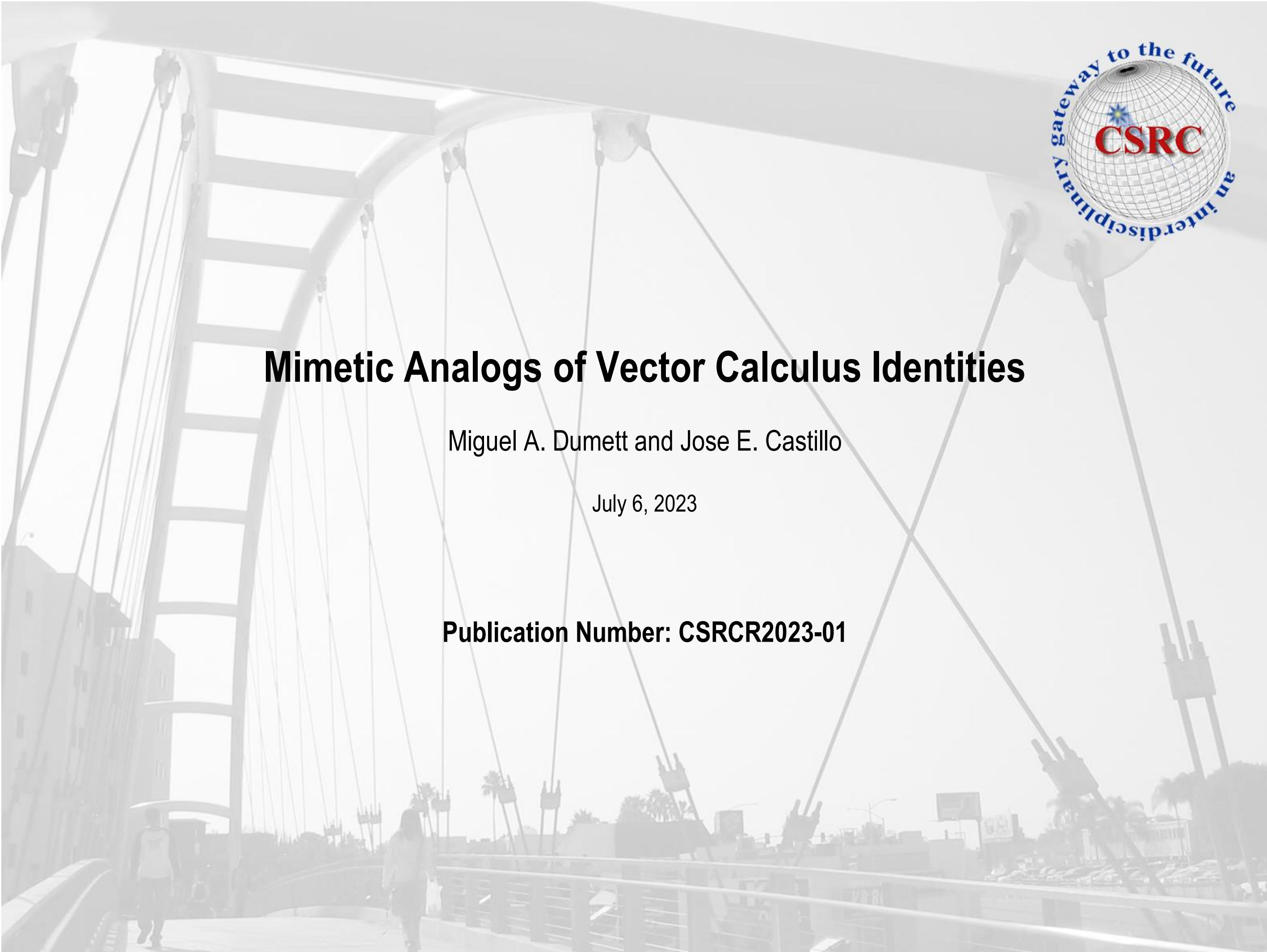

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Mimetic Analogs of Vector Calculus Identities *

Miguel A. Dumett † Jose E. Castillo ‡

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Abstract

In this paper we present a complete derivation of the three dimensions (3D) mimetic difference divergence, gradient, inner product weights and interpolation operators, using as an example the Corbino-Castillo mimetic method. In addition, we demonstrate in what sense these operators satisfy discrete analogs of 3D vector calculus identities.

1 Introduction

The main goal of this paper is to build mimetic difference discrete analogs of some vector calculus identities. This effort requires, besides the high-order divergence, gradient and Laplacian mimetic operators introduced in [1], [2], [5], the utilization of adequate high-order 3D interpolation operators exhibited in [7], as well as some identities derived from the mimetic discrete analog of the integration by parts (IBP) formula, and the 3D generalizations of these identities. These materials can be found in several references in the literature and most of it has not been previously published. This document shows a new full derivation of the Corbino-Castillo mimetic operators, as an example of mimetic differences, before constructing the discrete analogs in the integral sense. These vector calculus identities discrete analogs are independent of the mimetic method used and are valid provided a discrete analog of the IBP formula holds for the respective mimetic method.

In [5] Corbino-Castillo 1D, 2D, and 3D, mimetic divergence D, gradient G and Laplace L operators were introduced. In the same way as in [2], but with smaller band-with, and without free parameters, these operators are also defined on a staggered grid, meaning that discrete versions of scalar and vector fields are defined in different places of the grid. Similarly to the Castillo-Grone mimetic divergence, gradient and Laplace operators, they are constructed with constant (high-order) accuracy over interior as well as boundary grid points, and mimic the extended Gauss divergence theorem in 1D, or integration by parts, by utilizing diagonal positive definite weighted inner products P and Q.

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Indeed, satisfying a discrete analog of the IBP formula is central in the formulation of any of the existing mimetic difference methods. This property and their derived consequences are essential for proving energy conservation of the mimetic schemes. Unfortunately, the explicit requirement that mimetic operators should satisfy the IBP formula 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 exactly why initial versions of mimetic differences [4], [12], [9], [8], could only guarantee second-order accuracy of the IBP formula and but not higher-order and why [2] introduced matrices P and Q that induce inner products associated to the gradient and divergence mimetic operators, respectively.

Without the inner product induced by matrices P and Q, it is still possible to demonstrate discrete analogs of some of the vector calculus identities in their differential form but these are limited to second-order only.

To give a clearer idea of the contributions of these paper, details of the Corbino-Castillo mimetic differences already published follow.

Besides the introduction of matrices P and Q that guarantee a high-order discrete analog of the IBP formula, since matrix representations of the mimetic divergence and gradient operators hold the zero row sum property, discrete analog of the divergence of a constant vector field and the gradient of a constant scalar field are satisfied [2], [5], [1].

In addition, the staggered grid nature of the grid trigger the need of 1D constant high-order (at interior and boundary grid points) interpolations operators (from centers to faces and from faces to centers). These operators were introduced on [7].

The extension to 2D and 3D of the mimetic analogs of the extended Gauss divergence theorem requires the actual definition of high-dimensional versions not only of these constant high-order interpolation operators but also of the diagonal positive definite weighted inner products P and Q. The high-dimensional mimetic operators P and Q have been presented in talks and internal documents at the SDSU CSRC but never formally written. They are included in this document. They are created following ideas from [3].

The introduction of divergence and gradient mimetic operators on curvilinear coordinates [6] also demands the utilization of high-dimensional interpolation operators for the computation of the Jacobian and inverse Jacobian matrices [6].

The main contributions of this paper are:

1. Mimetic divergence and gradient operators are derived in a similar way as in [1], [2], [5], but the actual computation of their matrix representation entries utilizes formulas for the second row of the inverse of a Vandermonde matrix considered in [10].

2. Establishing the dependence on the number of cells of the weighted inner products entries of P and Q is discussed.

3. Explicit derivations from the IBP formula of certain identities of matrices D^TQ and G^TP are included. These properties are essential in the proof of energy conservation

of mimetic schemes by utilizing the interpolation operators.

4. Proof of mimetic discrete analogs of various vector calculus identities in integral form are given. In addition, discrete analogs of some vector calculus identities in differential form are included and are valid only for mimetic operators of order two.

In Section 2, the mimetic staggered grid and some notation for the related different grid subset points are presented.

In Section 3, formulas for computing directly the entries of the inverse of Vandermonde matrices according to [10] are introduced. These expressions are utilized for the calculation of the entries of the mimetic divergence and gradient operators. A similar approach is also explained when deriving mimetic interpolation operators (see Section 7). Calculating divergence and gradient operator entries via Taylor expansions was first suggested in [11]. Originally, mimetic operators matrices were obtained by differentiating Lagrange interpolation of scalar and vector fields (see, for example [4]).

In Section 4, the computation of divergence operators entries for accuracy orders $2, 4, 6, 8$, is shown. This is the first time Corbino-Castillo operator of degree 8 entries are displayed.

In Section 5, the computation of the gradient entries for accuracy orders $2, 4, 6, 8$, is exposed. This is the first time Corbino-Castillo operator of degree 8 entries are exhibited.

In Section 6, Laplace operators are exhibited.

In Section 7, interpolation operators are introduced. For the sake of completeness the material is taken from [7]. One row sum properties of these operators are also included.

In Section 8, the mimetic quadrature weights P and Q are presented. This discussion differs from [5] because of the realization that the entries of the corresponding matrix representations of operators P and Q depend on the number of cells. However, the difference between the P and Q entries in [5] and the one in the current document are very small and the calculation of energy conservation (when these operators are actually used) is not affected in practical terms.

In Section 9, the 1D mimetic boundary operators are presented and its extension to 3D is shown for the first time.

In Section 10, the extension to 3D of the extended Gauss divergence theorem is shown. This is the first time, this identity is displayed.

In Section 11, the demonstration of mimetic discrete analogs of some vector calculus identities in the integral form are exposed. As mentioned before, it turns out that vector calculus identities should be understood in the integral sense. This is because of the explicitly enforced mimetic discrete analog of the 1D IBP formula. This formula is utilized to introduce matrices P and Q and in this way to guarantee that a discrete analog of the IBP formula holds up to high-order of accuracy. This implicitly facilitates the demonstration of the integral version of vector calculus identities. However, it is possible to prove some of the vector calculus in their differential form, for example the gradient of a product of scalar fields, but these impose additional constraints on the mimetic operators, limiting for example the order of accuracy of some of the operators to two.

In section 12, conclusions and future work are described.

2 The staggered grid

In 1D, the number of cell centers and cell faces of a staggered grid is not the same. The same occurs in 2D and 3D, especially when the number of cells in each of the axis is different.

Since the divergence of a vector field is a scalar field, it is expected that mimetic matrices that represent discrete analogs of the divergence operator, on a staggered grid, are not square. Similarly, since the gradient of a scalar field is a vector field, it is also expected that the mimetic matrices that represent discrete analogs, on a staggered grid, of the gradient operator are not square.

As an example, consider in Figure 1, a two-dimensional uniformly staggered grid with five cells along the x-axis and four cells along the y-axis is displayed.

Scalar fields are defined on black dot places. In addition, the first component of vector fields are defined on the horizontal black segments while vector fields second components are defined on the vertical red segments.

Observe that the input data of a mimetic divergence operator is located on the horizontal and vertical black segments while its output is located at the black dots that are not on the boundary, since it is not possible to compute the continuous divergence on the boundary of a domain.

In addition, the input data for a mimetic gradient operator is located at the black dots and its output is located at the horizontal black segments (for the first component of the gradient) and at the vertical black segments (for the second component of the gradient).

To facilitate the definition of divergence and gradient operators on the d-dimensional Cartesian grid

$$\Pi_{i=1}^{d}[a_i, b_i] = [a_1, b_1] \times \cdots \times [a_d, b_d],$$

define

1. m_i the number of cells along the x_i axes, with mesh size $h_i = \frac{b_i - a_i}{m_i}$, $i = 1, \cdots, d$.

2. the x_i-Grid:

$$X^i = \left\{ x_j^i = a_i + \frac{j h_i}{2},\ j = 0, 1, \cdots, 2\, m_i \right\}, \qquad i = 1, \cdots, d.$$

3. the x_i-Nodes:

$$N^i = \left\{ x_j^i = a_i + j h_i,\ j = 0, 1, \cdots, m_i \right\}, \qquad i = 1, \cdots, d.$$

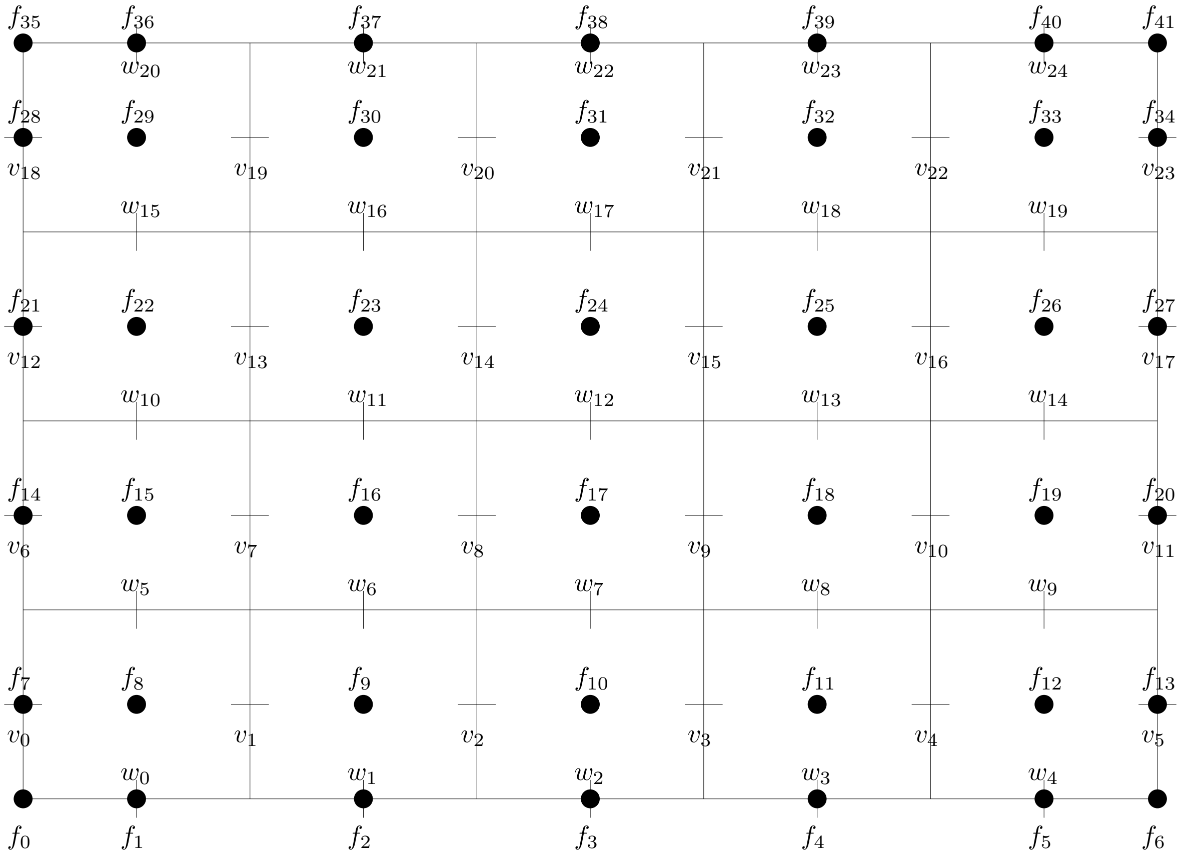

Figure 1: A staggered grid with 5 horizontal cells and 4 vertical cells.

4. the x_i-Centers:

$$C^i = \left\{ x^i_j = a_i + \frac{(2j-1)h_i}{2},\, j = 1, \cdots, m_i \right\}, \qquad i = 1, \cdots, d.$$

5. the x_i-Centers and Boundary:

$$S^i = C^i \cup \{-1, 1\}, \qquad i = 1, \cdots, d.$$

6. The grid: $X = X^1 \times \cdots \times X^d$.

7. The centers and boundary: $S = S^1 \times \cdots \times S^d$.

8. The nodes: $N = \cup_{i=1}^{d} (N^1 \times \cdots \times N^{i-1} \times S^i \times N^{i+1} \times \cdots \times N^d)$.

In this way, the mimetic divergence D and gradient G operators are defined as linear transformations as

$$D : N \to S, \qquad G : S \to N.$$

3 Computing mimetic operators without inverting matrices

The construction of Corbino-Castillo mimetic operators is facilitated by inverting a Vandermonde matrix. The construction of high-order divergence and gradient mimetic operators require the inversion of Vandermonde matrices, which might have large condition numbers. Software packages like MATLAB, even when utilizing *format rat*, introduce numerical errors when computing high-order versions of these operators.

Fortunately, [10] introduces one algorithm that computes entries of the inverse of Vandermonde matrices without inverting them. The method is as follows.

Given $p \in \mathbb{Z}^+$ real numbers $c_1, \cdots, c_p$, the associated Vandermonde matrix is given by

$$\mathbb{V} = \mathbb{V}(c_1, \cdots, c_p) = \begin{pmatrix} 1 & c_1 & c_1^2 & \cdots & c_1^{p-1} \\ 1 & c_2 & c_2^2 & \cdots & c_2^{p-1} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & c_p & c_p^2 & \cdots & c_p^{p-1} \end{pmatrix}.$$

The vector $c = (c_1, \cdots, c_p)$ is called the generator of the Vandermonde matrix $\mathbb{V}$.

The entry (i, j), $1 \leq i,\ j \leq p$, of its inverse $\mathbb{V}^{-1}$ is given by:

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

One can notice that in [10] there are several typos in the 4×4 example given.[1]

To enforce a constant degree of accuracy for its divergence and gradient operators, the derivation of the Corbino-Castillo mimetic coefficients $(q_1, \cdots, q_p)$, require the solution of several Vandermonde systems (with the appropriate generators) of the form

$$[q_1, \cdots, q_p]\ \mathbb{V}(c_1, \cdots, c_p) = [0, 1, 0, \cdots, 0],$$

[1] In page 210, the second row of the inverse of the Vandermonde matrix should be

$$\left[\frac{-(c_2c_3 + c_2c_4 + c_3c_4)}{(c_4 - c_1)(c_3 - c_1)(c_2 - c_1)}, \frac{c_1c_3 + c_1c_4 + c_3c_4}{(c_4 - c_2)(c_3 - c_2)(c_2 - c_1)}, \frac{-(c_1c_2 + c_1c_4 + c_2c_4)}{(c_4 - c_3)(c_3 - c_2)(c_3 - c_1)}, \frac{c_1c_2 + c_1c_3 + c_2c_3}{(c_4 - c_3)(c_4 - c_2)(c_4 - c_1)}\right],$$

instead of the one shown in that paper. There might be other typos in rows three and four since only rows one and two were verified.

and hence

$$[q_1, \cdots, q_p] = [0, 1, 0, \cdots, 0]\, \mathbb{V}^{-1}(c_1, \cdots, c_p) = \mathbb{V}^{-1}_{2,:}(c_1, \cdots, c_p),$$

where $\mathbb{V}^{-1}_{2,:}$ is the second row of the inverse of the Vandermonde matrix $\mathbb{V}$.

4 The divergence operators

The Corbino-Castillo 1D divergence operators D are defined as

$$D : N^1 \to S^1.$$

are are represented by matrices of order $(N+2) \times (N+1)$ with N the number of cells.

Divergence matrices first and last rows entries are zero because it is assumed that, the spatial domain of the PDE for which the discrete analog of the continuous divergence operator is restricted to a closed interval $[a, b]$, and hence the divergence operator is not defined on the interval boundaries.

However, if the spatial-temporal PDE domain strictly includes the interval $[a, b]$ the first and last rows of the discrete analog of the divergence operator are not zero. This allows the possibility of defining expanded divergence operators (see the next subsections). They do not appear in [5].

In addition, the divergence of a constant vector field should be zero. Since mimetic operators for dimensions greater than one are generated via Kronecker products of the corresponding 1D operators and other simple matrices, one just needs to impose the zero row sum property in 1D, or equivalently,

$$\sum_{j=1}^{N+1} D_{i,j} = 0. \tag{1}$$

Furthermore, assume one wants to compute a discrete analog of order of accuracy k (even) of the 1D divergence at $x^1_j = a_1 + \frac{(2j-1)h_1}{2} \in C^1$, for some j, $1 \le j \le m_1$. Assume that x_j (omitting all upper indices since it is the one-dimensional version of the staggered grid) is an interior cell center, in the sense that all cell faces

$$n_i = x_j + \frac{(2i+1)h}{2}, \qquad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1,$$

are in N, or equivalently, all $\frac{k}{2}$ cell faces to the left and $\frac{k}{2}$ cells faces to the right of $x_j \in C$, are in N. For each of the cell faces n_i (data that is part of the discrete version V of a vector field $\vec{v}$, since the information is at the faces) of such interior cell center x_j, one can compute the discrete analog of the divergence at the (interior) cell center x_j (output that is part of the discrete version DV of the divergence scalar field $\nabla \cdot \vec{v}$) by performing Taylor expansions of the 1D vector field $\vec{v}$ (omitting the arrow since it is one-dimensional)

$$v(n_i) = \sum_{l=0}^{k} \frac{1}{l!} (n_i - x_j)^l v^{(l)}(x_j) + \mathcal{O}(h^{k+1}), \quad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1.$$

If one collects all k identities $v(n_i)$ into a vector of length k one obtains

$$\begin{bmatrix} v(n_{-\frac{k}{2}}) \\ v(n_{-\frac{k}{2}+1}) \\ \vdots \\ v(n_{\frac{k}{2}-2}) \\ v(n_{\frac{k}{2}-1}) \end{bmatrix} = \begin{bmatrix} 1 & \frac{(-k+1)h}{2} & \left(\frac{(-k+1)h}{2}\right)^2 & \cdots & \left(\frac{(-k+1)h}{2}\right)^k \\ 1 & \frac{(-k+3)h}{2} & \left(\frac{(-k+3)h}{2}\right)^2 & \cdots & \left(\frac{(-k+3)h}{2}\right)^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \frac{(k-3)h}{2} & \left(\frac{(k-3)h}{2}\right)^2 & \cdots & \left(\frac{(k-3)h}{2}\right)^k \\ 1 & \frac{(k-1)h}{2} & \left(\frac{(k-1)h}{2}\right)^2 & \cdots & \left(\frac{(k-1)h}{2}\right)^k \end{bmatrix} \begin{bmatrix} v(x_j) \\ v^{'}(x_j) \\ \cdots \\ v^{(k-1)}(x_j) \\ v^{(k)}(x_j) \end{bmatrix} + \mathcal{O}(h^{k+1})$$

If one wants that these expansions produce a k-th accuracy order estimate of $v^{'}(x_j)$ then one needs to solve

$$\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right) \begin{bmatrix} v(x_j) \\ v^{'}(x_j) \\ \cdots \\ v^{(k-1)}(x_j) \\ v^{(k)}(x_j) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad (2)$$

where $\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$ is a Vandermonde matrix with generator $c = \left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$.

For the non-interior cell centers a similar approach applies. In the Corbino-Castillo operators, each non-interior cell center x_j is computed utilizing the values of discrete version of $\vec{v}$ at the nearest boundary and the nearest k cell faces to the specified boundary. Solving (2), with an appropriate generator, provides the numerical scheme for the divergence discrete analog at x_j.

Observe that, because of the reflexivity of D with respect to the center of interval $[a, b]$ and the symmetry with respect to the boundary of the same interval, then

$$D_{N+3-i,N+2-j} = -D_{i,j}, \qquad 1 \leq i \leq N+2, \qquad 1 \leq j \leq N+1.$$

Hence, it is only needed to specify the first $\lceil \frac{N}{2} \rceil + 1$ rows of D.

For $k=2$, the generator of the interior scheme is $d_2 = [-\frac{1}{2}, \frac{1}{2}]$.

$$D^{(2)} = \frac{1}{h}\begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}.$$

For $k=4$, the generator for the interior scheme of the divergence is $d_4 = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}]$. The generator associated to the divergence near the boundary is $d_{41} = [-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$.

$$D^{(4)} = \frac{1}{h}\begin{bmatrix} -\frac{11}{12} & \frac{17}{24} & \frac{3}{8} & -\frac{5}{24} & \frac{1}{24} & 0 & \cdots \\ \frac{1}{24} & -\frac{9}{8} & \frac{9}{8} & -\frac{1}{24} & 0 & \cdots & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}.$$

For $k=6$, the generator for the interior scheme of the divergence is $d_6 = [-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}]$. The generators associated to the interpolation near the boundary are $d_{61} = [-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$, and $d_{62} = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}]$.

$$D^{(6)} = \frac{1}{h}\begin{bmatrix} -\frac{1627}{1920} & \frac{211}{640} & \frac{59}{48} & -\frac{235}{192} & \frac{91}{128} & -\frac{443}{1920} & \frac{31}{960} & 0 & \cdots \\ \frac{31}{960} & -\frac{687}{640} & \frac{129}{128} & \frac{19}{192} & -\frac{3}{32} & \frac{21}{640} & -\frac{3}{640} & 0 & \cdots \\ -\frac{3}{640} & \frac{25}{384} & -\frac{75}{64} & \frac{75}{64} & -\frac{25}{384} & \frac{3}{640} & 0 & \cdots & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \end{bmatrix}.$$

For $k=8$, the generator for the interior scheme of the divergence is $d_8 = [-\frac{7}{2}, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$. The generators associated to the divergence near the boundary are $d_{81} = [-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}, \frac{15}{2}]$, and $d_{82} = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}]$, and $d_{83} = [-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$.

$$D^{(8)} = \frac{1}{h}\begin{bmatrix} -\frac{1423}{1792} & -\frac{491}{7168} & \frac{7753}{3072} & -\frac{18509}{5120} & \frac{3535}{1024} & -\frac{2279}{1024} & \frac{953}{1024} & -\frac{1637}{7168} & \frac{2689}{107520} & 0 & \cdots \\ \frac{2689}{107520} & -\frac{36527}{35840} & \frac{4259}{5120} & \frac{6497}{15360} & -\frac{475}{1024} & \frac{1541}{5120} & -\frac{639}{5120} & \frac{1087}{35840} & -\frac{59}{17920} & 0 & \cdots \\ -\frac{59}{17920} & \frac{1175}{21504} & -\frac{1165}{1024} & \frac{1135}{1024} & \frac{25}{3072} & -\frac{251}{5120} & \frac{25}{1024} & -\frac{45}{7168} & \frac{5}{7168} & 0 & \cdots \\ \frac{5}{7168} & -\frac{49}{5120} & \frac{245}{3072} & -\frac{1225}{1024} & \frac{1225}{1024} & -\frac{245}{3072} & \frac{49}{5120} & -\frac{5}{7168} & 0 & \cdots & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \end{bmatrix}.$$

4.1 The 2D and 3D divergence operators

For Cartesian grids $[a_1, b_1] \times [a_2, b_2]$ and $[a_1, b_1] \times [a_2, b_2] \times [a_3, b_3]$ with m, n, o cells in the x, y, z-axes, respectively, they are constructed by utilizing the Kronecker product $\otimes$.

The 2D divergence operators $D^{(k)}_{xy}$ of k-th order are given by

$$D^{(k)}_{xy} = [D^{(k)}_{xy,1}, \quad D^{(k)}_{xy,2}] = [\hat{I}_n \otimes D^{(k)}_x, \quad D^{(k)}_y \otimes \hat{I}_m],$$

and the 3D divergence operators $D^{(k)}_{xyz}$ of k-th order are given by

$$D^{(k)}_{xyz} = [D^{(k)}_{xyz,1}, \quad D^{(k)}_{xyz,2} \quad D^{(k)}_{xyz,3}] = [\hat{I}_o \otimes \hat{I}_n \otimes D^{(k)}_x, \quad \hat{I}_o \otimes D^{(k)}_y \otimes \hat{I}_m, \quad D^{(k)}_z \otimes \hat{I}_n \otimes \hat{I}_m],$$

where $D^{(k)}_p$ is the 1D divergence operator along the p-axis, and

$$\hat{I}_q = \begin{bmatrix} 0_{1\times q} \\ I_{q\times q} \\ 0_{1\times q} \end{bmatrix},$$

with $I_{q\times q}$ is the $q \times q$ identity matrix.

Notice that (1) implies

$$D_{xyz}\mathbb{1} = \vec{0}.$$

5 The gradient operators

The Corbino-Castillo 1D gradient operators G are defined as linear transformations

$$G : S^1 \to N^1,$$

and are represented by matrices of order $(N+1)\times(N+2)$ with N the number of cells.

The gradient of a constant scalar field should be zero. Since mimetic operators for dimensions greater than one are generated via Kronecker products of the corresponding 1D operators and other simple matrices, one just needs to impose this zero row sum property in 1D, or equivalently,

$$\sum_{j=1}^{N+1} G_{i,j} = 0. \tag{3}$$

Furthermore, assume one wants to compute a discrete analog of order of accuracy k (even) of the 1D gradient at $x_j^1 = a_1 + \frac{jh_1}{2} \in N^1$, for some j, $0 \le j \le m_1$. Assume that x_j (omitting all upper indices since it is the one-dimensional version of the staggered grid) is an interior cell face, in the sense that all cell centers

$$c_i = x_j + \frac{(2i+1)h}{2}, \qquad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1,$$

are in C, or equivalently, all $\frac{k}{2}$ cell centers to the left and $\frac{k}{2}$ cells centers to the right of $x_j \in N$, are in C. For each of the cell center c_i (data that is part of the discrete version F of a scalar field f, since the information is at the centers) of such interior cell face x_j one can compute the discrete analog of the gradient at the (interior) cell face x_j (output that is part of the discrete version Gf of the gradient vector field ∇f) by performing Taylor expansions of the 1D vector field f

$$f(c_i) = \sum_{l=0}^{k} \frac{1}{l!}(c_i - x_j)^l f^{(l)}(x_j) + \mathcal{O}(h^{k+1}), \quad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1.$$

If one collects all k identities $f(c_i)$ into a vector of length k one obtains

$$\begin{bmatrix} f(c_{-\frac{k}{2}}) \\ f(c_{-\frac{k}{2}+1}) \\ \vdots \\ f(c_{\frac{k}{2}-2}) \\ f(c_{\frac{k}{2}-1}) \end{bmatrix} = \begin{bmatrix} 1 & \frac{(-k+1)h}{2} & \left(\frac{(-k+1)h}{2}\right)^2 & \cdots & \left(\frac{(-k+1)h}{2}\right)^k \\ 1 & \frac{(-k+3)h}{2} & \left(\frac{(-k+3)h}{2}\right)^2 & \cdots & \left(\frac{(-k+3)h}{2}\right)^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \frac{(k-3)h}{2} & \left(\frac{(k-3)h}{2}\right)^2 & \cdots & \left(\frac{(k-3)h}{2}\right)^k \\ 1 & \frac{(k-1)h}{2} & \left(\frac{(k-1)h}{2}\right)^2 & \cdots & \left(\frac{(k-1)h}{2}\right)^k \end{bmatrix} \begin{bmatrix} f(x_j) \\ f'(x_j) \\ \cdots \\ f^{(k-1)}(x_j) \\ f^{(k)}(x_j) \end{bmatrix} + \mathcal{O}(h^{k+1})$$

If one wants that these expansions produce a k-th accuracy order estimate of $f'(x_j)$ then one needs to solve

$$\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right) \begin{bmatrix} f(x_j) \\ f'(x_j) \\ \cdots \\ f^{(k-1)}(x_j) \\ f^{(k)}(x_j) \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{4}$$

where $\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$ is a Vandermonde matrix with generator $c = \left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$.

Because each interior cell face is surrounded by two cell centers and each interior cell center is surrounded by two cell faces then systems (4) and (2) are exactly the same, and hence the scheme for a discrete analog of the divergence at an interior cell center is the same as the scheme for a discrete analog of the gradient at an interior cell face.

For the non-interior cell faces a similar approach applies. In the Corbino-Castillo operators, each non-interior cell face x_j is computed utilizing the values of discrete version of scalar field f at the nearest boundary and the nearest k cell centers to the specified boundary. Solving (4), with an appropriate generator, provides the numerical scheme for the gradient discrete analog at x_j.

Because of the reflexivity of G with respect to the center of interval $[a, b]$, one has that

$$G_{N+2-i,N+3-j} = -G_{i,j}, \qquad 1 \le i \le N+1, \qquad 1 \le j \le N+2.$$

Hence, it is only needed to specify the first $\lceil \frac{N+1}{2} \rceil$ rows of G.

For $k = 2$, the generator of the interior scheme is $g_2 = [-\frac{1}{2}, \frac{1}{2}]$. The generator associated to the gradient near the boundary is $g_{21} = [0, \frac{1}{2}, \frac{3}{2}]$.

$$G^{(2)} = \frac{1}{h}\begin{bmatrix} -\frac{8}{3} & 3 & -\frac{1}{3} & & & \\ & -1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & -1 & 1 & \\ & & & \frac{1}{3} & -3 & \frac{8}{3} \end{bmatrix}$$

For $k = 4$, the generator for the interior scheme of the gradient is $g_4 = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}]$. The generator associated to the interpolation near the boundary is $g_{41} = [0, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$ and $g_{42} = [-1, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}]$.

$$G^{(4)} = \frac{1}{h}\begin{bmatrix} -\frac{352}{105} & \frac{35}{8} & -\frac{35}{24} & \frac{21}{40} & -\frac{5}{56} & 0 & \cdots \\ \frac{16}{105} & -\frac{31}{24} & \frac{29}{24} & -\frac{3}{40} & \frac{1}{168} & 0 & \cdots \\ 0 & \frac{1}{24} & -\frac{9}{8} & \frac{9}{8} & -\frac{1}{24} & 0 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}$$

For $k = 6$, the generator for the interior scheme of the gradient is $g_6 = [-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}]$. The generators associated to the gradient near the boundary are $g_{61} = [0, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$, and $g_{62} = [-1, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}]$, and $g_{63} = [-2, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$.

$$G^{(6)} = \frac{1}{h} \begin{bmatrix} -\frac{13016}{3465} & \frac{693}{128} & -\frac{385}{128} & \frac{693}{320} & -\frac{495}{448} & \frac{385}{1152} & -\frac{63}{1408} & 0 & \cdots & \\ \frac{496}{3465} & -\frac{811}{640} & \frac{449}{384} & -\frac{29}{960} & -\frac{11}{448} & \frac{13}{1152} & -\frac{37}{21120} & 0 & \cdots & \\ -\frac{8}{385} & \frac{179}{1920} & -\frac{153}{128} & \frac{381}{320} & -\frac{101}{1344} & \frac{1}{128} & -\frac{3}{7040} & 0 & \cdots & \\ & -\frac{3}{640} & \frac{25}{384} & -\frac{75}{64} & \frac{75}{64} & -\frac{25}{384} & \frac{3}{640} & 0 & \cdots & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \end{bmatrix}.$$

For $k = 8$, the generator for the interior scheme of the gradient is $g_8 = [-\frac{7}{2}, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$. The generators associated to the gradient near the boundary are $g_{81} = [0, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}, \frac{15}{2}]$, and $g_{82} = [-1, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}]$, and $g_{83} = [-2, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$, and $g_{84} = [-3, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}]$.

$$G^{(8)} = \frac{1}{h} \begin{bmatrix} -\frac{182144}{45045} & \frac{6435}{1024} & -\frac{5055}{1024} & \frac{27027}{5120} & -\frac{32175}{7168} & \frac{25025}{9216} & -\frac{12285}{11264} & \frac{3465}{13312} & -\frac{143}{5120} & 0 & \cdots & \\ \frac{86048}{675675} & -\frac{131093}{107520} & \frac{49087}{46080} & \frac{10973}{76800} & -\frac{4597}{21504} & \frac{4019}{27648} & -\frac{10331}{168960} & \frac{2983}{199680} & -\frac{2621}{1612800} & 0 & \cdots & \\ -\frac{3776}{225225} & \frac{8707}{107520} & -\frac{17947}{15360} & \frac{29319}{25600} & -\frac{533}{21504} & -\frac{263}{9216} & \frac{903}{56320} & -\frac{283}{66560} & \frac{257}{537600} & 0 & \cdots & \\ \frac{32}{9009} & -\frac{543}{35840} & \frac{265}{3072} & -\frac{1233}{1024} & \frac{8625}{7168} & -\frac{775}{9216} & \frac{639}{56320} & -\frac{15}{13312} & \frac{1}{21504} & 0 & \cdots & \\ & \frac{5}{7168} & -\frac{49}{5120} & \frac{245}{3072} & -\frac{1225}{1024} & \frac{1225}{1024} & -\frac{245}{3072} & \frac{49}{5120} & -\frac{5}{7168} & 0 & \cdots & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & & \end{bmatrix}.$$

5.1 The 2D and 3D gradient operators

For a Cartesian grid with m, n, o cells in the x, y, z-axes, respectively, they are constructed by utilizing the Kronecker product $\otimes$.

The 2D gradient operators $G^{(k)}_{xy}$ of k-th order are given by

$$G^{(k)}_{xy} = \begin{bmatrix} G^{(k)}_{xy,1} \\ G^{(k)}_{xy,2} \end{bmatrix} = \begin{bmatrix} \hat{I}^T_n \otimes G^{(k)}_x \\ G^{(k)}_y \otimes \hat{I}^T_m \end{bmatrix}$$

and the 3D gradient operators $G^{(k)}_{xyz}$ of k-th order are given by

$$G^{(k)}_{xyz} = \begin{bmatrix} G^{(k)}_{xyz,1} \\ G^{(k)}_{xyz,2} \\ G^{(k)}_{xyz,3} \end{bmatrix} = \begin{bmatrix} \hat{I}^T_o \otimes \hat{I}^T_n \otimes G^{(k)}_x \\ \hat{I}^T_o \otimes G^{(k)}_y \otimes \hat{I}^T_m \\ G^{(k)}_z \otimes \hat{I}^T_n \otimes \hat{I}^T_m \end{bmatrix}$$

where $G_p^{(k)}$ is the 1D gradient operator along the p-axis, and

$$\hat{I}_q = \begin{bmatrix} 0_{1\times q} \\ I_{q\times q} \\ 0_{1\times q} \end{bmatrix},$$

with $I_{q\times q}$ is the $q \times q$ identity matrix.

Notice that (3) implies

$$G_{xyz}\mathbb{1} = 0. \tag{5}$$

6 The Laplace operators

For a Cartesian grid with m, n, o cells in the x, y, z-axes, respectively, the Castillo-Corbino Laplace operators L are defined as products of the corresponding divergence and gradient operators. Therefore,

$$\begin{aligned} L_x^{(k)} &= D_x^{(k)}\, G_x^{(k)}, \\ L_{xy}^{(k)} &= D_{xy}^{(k)}\, G_{xy}^{(k)}, \\ L_{xyz}^{(k)} &= D_{xyz}^{(k)}\, G_{xyz}^{(k)}. \end{aligned}$$

7 The interpolation operators

The staggered grid utilized in the Corbino-Castillo mimetic divergence and gradient operators may sometimes cause that quantities that need to be added of multiplied are defined on different places (centers or faces). For example, consider the nonlinear term $u\,\nabla u$ in the Navier-Stokes equation. Some of these quantities need to be interpolated to make the operation in question feasible. These interpolation operators must have the same order of accuracy as the mimetic operators involved.

In [10] an exact algorithm for the computation of the inverse of the Vandermonde matrix is given. The first row of it is what is needed for finding interpolation operators (derivative of zero order) of orders $k = 2, 4, 6, 8$ exactly. These interpolation operators guarantee that the divergence and gradient interpolation operators will have data in the required places.

The derivation of the Corbino-Castillo interpolation operators for any dimensions can be found in [7]. From [10], one can infer that if the generator of the Vandermonde matrix is given by

$$c = [c_1, \cdots, c_m],$$

then the first row of the inverse of the respective Vandermode matrix (which corresponds to the row of interest for the interpolation operator) is given by

$$\left[\frac{p_1}{d_1}, \cdots, \frac{p_m}{d_m}\right],$$

where

$$p_i = \frac{p}{c_i}, \qquad p = \prod_{i=1}^{m} c_i, \qquad d_i = \prod_{j \neq i} (c_j - c_i).$$

7.1 The 1D divergence interpolation operators

The Corbino-Castillo 1D divergence interpolation operators I_D are transformations

$$I_D : S^1 \to N^1,$$

represented by matrices of order $(N+1) \times (N+2)$ with N the number of cells. These operators move the data from cell centers to faces before applying the divergence operator.

In addition, the divergence interpolation of a constant vector field should be the same constant. Since mimetic operators for dimensions greater than one are generated via Kronecker products of the corresponding 1D operators and other simple matrices, one just needs to impose the one row sum property in 1D, or equivalently,

$$\sum_{j=1}^{N+2} (I_D)_{i,j} = 1. \tag{6}$$

Furthermore, assume one wants to interpolate with order of accuracy k (even) at the cell face $x_j^1 = a_1 + \frac{jh_1}{2} \in N^1$, for some j, $0 \leq j \leq m_1$. Assume that x_j (omitting all upper indices since it is the one-dimensional version of the staggered grid) is an interior cell face, in the sense that all cell centers

$$c_i = x_j + \frac{(2i+1)h}{2}, \qquad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1,$$

are in C, or equivalently, all $\frac{k}{2}$ cell centers to the left and $\frac{k}{2}$ cells centers to the right of $x_j \in N$, are in C. For each of the cell center c_i (data that is part of the discrete version V of a vector field $\vec{v}$, since the information is at the centers) of such interior cell face x_j one can perform a Taylor expansions of the 1D vector field $\vec{v}$

$$v(c_i) = \sum_{l=0}^{k} \frac{1}{l!} (c_i - x_j)^l v^{(l)}(x_j) + \mathcal{O}(h^{k+1}), \quad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1.$$

If one collects all k identities $v(c_i)$ into a vector of length k one obtains

$$\begin{bmatrix} v(c_{-\frac{k}{2}}) \\ v(c_{-\frac{k}{2}+1}) \\ \vdots \\ v(c_{\frac{k}{2}-2}) \\ v(c_{\frac{k}{2}-1}) \end{bmatrix} = \begin{bmatrix} 1 & \frac{(-k+1)h}{2} & \left(\frac{(-k+1)h}{2}\right)^2 & \cdots & \left(\frac{(-k+1)h}{2}\right)^k \\ 1 & \frac{(-k+3)h}{2} & \left(\frac{(-k+3)h}{2}\right)^2 & \cdots & \left(\frac{(-k+3)h}{2}\right)^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \frac{(k-3)h}{2} & \left(\frac{(k-3)h}{2}\right)^2 & \cdots & \left(\frac{(k-3)h}{2}\right)^k \\ 1 & \frac{(k-1)h}{2} & \left(\frac{(k-1)h}{2}\right)^2 & \cdots & \left(\frac{(k-1)h}{2}\right)^k \end{bmatrix} \begin{bmatrix} v(x_j) \\ v'(x_j) \\ \cdots \\ v^{(k-1)}(x_j) \\ v^{(k)}(x_j) \end{bmatrix} + \mathcal{O}(h^{k+1})$$

If one wants that these expansions produce a k-th accuracy order estimate of $v(x_j)$ then one needs to solve

$$\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)\begin{bmatrix} v(x_j) \\ v^{'}(x_j) \\ \cdots \\ v^{(k-1)}(x_j) \\ v^{(k)}(x_j) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix} \tag{7}$$

where $\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$ is a Vandermonde matrix with generator $c = \left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$.

Observe that the Vandermonde matrices of (4), (2), and (7) are exactly the same, but the right hand side of (7) is different.

For the non-interior cell faces a similar approach applies. In the Corbino-Castillo operators, each non-interior cell face x_j is computed utilizing the values of discrete version of vector field $\vec{v}$ at the nearest boundary and the nearest k cell centers to the specified boundary. Solving (7), with an appropriate generator, provides the numerical scheme for the divergence interpolation operator at x_j.

Because of the reflexivity of I_D with respect to the center of interval $[a, b]$, one has that

$$(I_D)_{N+2-i,N+3-j} = (I_D)_{i,j}, \qquad 1 \le i \le N+1, \qquad 1 \le j \le N+2.$$

Hence, it is only needed to specify the first $\lceil \frac{N+1}{2} \rceil$ rows of I_D.

For $k = 2$, the generator of the divergence interpolator $I_D^{(2)}$ is $d_2 = [-\frac{1}{2}, \frac{1}{2}]$ and

$$I_D^{(2)} = \frac{1}{2}\begin{bmatrix} 2 & & & & & \\ & 1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & 1 & \\ & & & & & 2 \end{bmatrix}.$$

For $k = 4$, the generator for the interior scheme of the divergence interpolator $I_D^{(4)}$ is $d_4 = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}]$. The generator associated to the interpolation near the boundary is $d_{41} = [-1, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}]$. Thus, the non-zero entries of $I_D^{(4)}$ are given by

$$I_D^{(4)} = \frac{1}{112}\begin{bmatrix} 112 & & & & & & \\ -16 & 70 & 70 & -14 & 2 & & \\ & -7 & 63 & 63 & -7 & & \\ & & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}.$$

For $k = 6$, the generator for the interior scheme of the divergence interpolator $I_D^{(6)}$ is $d_6 = [-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}]$. The generators associated to the interpolation near the boundary are $d_{61} = [-1, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}]$, and $d_{62} = [-2, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$. Thus, the non-zero entries of $I_D^{(6)}$ are given by

$$I_D^{(6)} = \frac{1}{8448}\begin{bmatrix} 8448 & & & & & & & \\ -768 & 4158 & 6930 & -2772 & 1188 & -330 & 42 & \\ 256 & -924 & 4620 & 5544 & -1320 & 308 & -36 & \\ & 99 & -825 & 4950 & 4950 & -825 & 99 & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

For $k = 8$, the generator for the interior scheme of the divergence interpolator $I_D^{(8)}$ is $g = [-\frac{7}{2}, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$. The generators associated to the interpolation near the boundary are $g = [-1, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}]$, and $g = [-2, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$, and $g = [-3, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}]$. Thus, the non-zero entries of $I_D^{(8)}$ are given by

$$I_D^{(8)} = \begin{bmatrix} 1 & & & & & & & & & & \\ -\frac{1}{15} & \frac{429}{1024} & \frac{1001}{1024} & -\frac{3003}{5120} & \frac{429}{1024} & -\frac{715}{3072} & \frac{91}{1024} & -\frac{21}{1024} & \frac{11}{5120} & & \\ \frac{1}{65} & -\frac{33}{512} & \frac{231}{512} & \frac{2079}{2560} & -\frac{165}{512} & \frac{77}{512} & -\frac{27}{512} & \frac{77}{6656} & -\frac{3}{2560} & & \\ -\frac{1}{143} & \frac{27}{1024} & -\frac{105}{1024} & \frac{567}{1024} & \frac{675}{1024} & -\frac{175}{1024} & \frac{567}{11264} & -\frac{135}{13312} & \frac{1}{1024} & & \\ & -\frac{5}{2048} & \frac{49}{2048} & -\frac{245}{2048} & \frac{1225}{2048} & \frac{1225}{2048} & -\frac{245}{2048} & \frac{49}{2048} & -\frac{5}{2048} & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}.$$

7.1.1 The 2D and 3D divergence interpolation operators

For a Cartesian grid with m, n, o cells in the x, y, z-axes, respectively, they are constructed by utilizing the Kronecker product $\otimes$.

The 2D divergence interpolation operators $(I_D)_{xy}^{(k)}$ of k-th order are given by

$$(I_D)_{xy}^{(k)} = \begin{bmatrix} (I_D)_{xy,1}^{(k)} & \\ & (I_D)_{xy,2}^{(k)} \end{bmatrix} = \begin{bmatrix} \hat{I}_n^T \otimes (I_D)_x^{(k)} & \\ & (I_D)_y^{(k)} \otimes \hat{I}_m^T \end{bmatrix},$$

and the 3D divergence interpolation operators $(I_D)^{(k)}_{xyz}$ of k-th order are given by

$$
\begin{aligned}
(I_D)^{(k)}_{xyz} &= \begin{bmatrix} (I_D)^{(k)}_{xyz,1} & & \\ & (I_D)^{(k)}_{xyz,2} & \\ & & (I_D)^{(k)}_{xyz,3} \end{bmatrix} \\
&= \begin{bmatrix} \hat{I}_o^T \otimes \hat{I}_n^T \otimes (I_D)^{(k)}_x & & \\ & \hat{I}_o^T \otimes (I_D)^{(k)}_y \otimes \hat{I}_m^T & \\ & & (I_D)^{(k)}_z \otimes \hat{I}_n^T \otimes \hat{I}_m^T \end{bmatrix},
\end{aligned}
$$

where $(I_D)^{(k)}_p$ is the 1D divergence interpolation operator along the p-axis, and

$$
\hat{I}_q = \begin{bmatrix} 0_{1\times q} \\ I_{q\times q} \\ 0_{1\times q} \end{bmatrix},
$$

with $I_{q\times q}$ is the $q \times q$ identity matrix.

Notice that (6) implies

$$
(I_D)_{xyz}\mathbb{1} = \mathbb{1}. \tag{8}
$$

7.2 The 1D gradient interpolation operators

The Corbino-Castillo 1D gradient interpolation operators I_G are transformations

$$
I_G : N^1 \to S^1,
$$

that are represented by matrices of order $(N+2) \times (N+1)$ with N the number of cells. The interpolation operator moves back the data from faces to centers after the gradient operator has been applied.

In addition, the gradient interpolation of a constant scalar field should be the same constant. Since mimetic operators for dimensions greater than one are generated via Kronecker products of the corresponding 1D operators and other simple matrices, one just needs to impose the one row sum property in 1D, or equivalently,

$$
\sum_{j=1}^{N+1} (I_G)_{i,j} = 1. \tag{9}
$$

Furthermore, assume one wants to compute interpolate with order of accuracy k (even) at the cell center $x^1_j = a_1 + \frac{(2j-1)h_1}{2} \in C^1$, for some j, $1 \le j \le m_1$. Assume that x_j (omitting all upper indices since it is the one-dimensional version of the staggered grid) is an interior cell center, in the sense that all cell faces

$$
n_i = x_j + \frac{(2i+1)h}{2}, \qquad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1,
$$

are in N, or equivalently, all $\frac{k}{2}$ cell faces to the left and $\frac{k}{2}$ cells faces to the right of $x_j \in C$, are in N. For each of the cell face n_i (data that is part of the discrete version f of a scalar field f, since the information is at the faces) of such interior cell center x_j one can perform a Taylor expansions of the 1D vector field $\vec{v}$ (omitting the arrow since it is one-dimensional)

$$f(n_i) = \sum_{l=0}^{k} \frac{1}{l!}(n_i - x_j)^l f^{(l)}(x_j) + \mathcal{O}(h^{k+1}), \quad i = -\frac{k}{2}, -\frac{k}{2}+1, \cdots, -1, 0, 1, \cdots, \frac{k}{2}-2, \frac{k}{2}-1.$$

If one collects all k identities $f(n_i)$ into a vector of length k one obtains

$$\begin{bmatrix} f(n_{-\frac{k}{2}}) \\ f(n_{-\frac{k}{2}+1}) \\ \vdots \\ f(n_{\frac{k}{2}-2}) \\ f(n_{\frac{k}{2}-1}) \end{bmatrix} = \begin{bmatrix} 1 & \frac{(-k+1)h}{2} & \left(\frac{(-k+1)h}{2}\right)^2 & \cdots & \left(\frac{(-k+1)h}{2}\right)^k \\ 1 & \frac{(-k+3)h}{2} & \left(\frac{(-k+3)h}{2}\right)^2 & \cdots & \left(\frac{(-k+3)h}{2}\right)^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \frac{(k-3)h}{2} & \left(\frac{(k-3)h}{2}\right)^2 & \cdots & \left(\frac{(k-3)h}{2}\right)^k \\ 1 & \frac{(k-1)h}{2} & \left(\frac{(k-1)h}{2}\right)^2 & \cdots & \left(\frac{(k-1)h}{2}\right)^k \end{bmatrix} \begin{bmatrix} v(x_j) \\ v'(x_j) \\ \cdots \\ v^{(k-1)}(x_j) \\ v^{(k)}(x_j) \end{bmatrix} + \mathcal{O}(h^{k+1})$$

If one wants that these expansions produce a k-th accuracy order estimate of $f(x_j)$ then one needs to solve

$$\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right) \begin{bmatrix} v(x_j) \\ v'(x_j) \\ \cdots \\ v^{(k-1)}(x_j) \\ v^{(k)}(x_j) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix} \tag{10}$$

where $\mathbb{V}\left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$ is a Vandermonde matrix with generator $c = \left(\frac{(-k+1)h}{2}, \frac{(-k+3)h}{2}, \cdots, \frac{(k-3)h}{2}, \frac{(k-1)h}{2}\right)$.

Observe that the Vandermonde matrices of (4), (2), (7), and (10) are exactly the same, and the right hand side of (7) and (10) are also the same.

For the non-interior cell centers a similar approach applies. In the Corbino-Castillo operators, each non-interior cell center x_j is computed utilizing the values of discrete version of f at the nearest boundary and the nearest k cell faces to the specified boundary. Solving (10), with an appropriate generator, provides the numerical scheme for the gradient interpolation operator at x_j.

Because of the reflexivity of I_G with respect to the center of interval $[a, b]$, one has that

$$(I_G)_{N+3-i,N+2-j} = (I_G)_{i,j}, \qquad 1 \le i \le N+2, \qquad 1 \le j \le N+1.$$

Hence, it is only needed to specify the first $\lceil \frac{N}{2} \rceil + 1$ rows of I_G.

For $k = 2$, the generator of the gradient interpolator $I_G^{(2)}$ is $g_2 = [-\frac{1}{2}, \frac{1}{2}]$ and

$$I_G^{(2)} = \frac{1}{2} \begin{bmatrix} 2 & & & \\ 1 & 1 & & \\ & \ddots & \ddots & \\ & & 1 & 1 \\ & & & 2 \end{bmatrix}.$$

For $k = 4$, the generator for the interior scheme of the gradient interpolator $I_G^{(4)}$ is $g_4 = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}]$. The generator associated to the interpolation near the boundary is $g_{41} = [-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$. Thus, the non-zero entries of $I_G^{(4)}$ are given by

$$I_G^{(4)} = \frac{1}{128} \begin{bmatrix} 128 & & & & & \\ 35 & 140 & -70 & 28 & -5 & \\ -8 & 72 & 72 & -8 & & \\ & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}.$$

For $k = 6$, the generator for the interior scheme of the gradient interpolator $I_G^{(6)}$ is $g_6 = [-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}]$. The generator associated to the interpolation near the boundary are $g_{61} = [-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$, and $g_{62} = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}]$. Thus, $I_G^{(6)}$ is given by

$$I_G^{(6)} = \frac{1}{1024} \begin{bmatrix} 1024 & & & & & & & \\ 231 & 1386 & -1155 & 924 & -495 & 154 & -21 & \\ -21 & 378 & 945 & -420 & 189 & -54 & 7 & \\ 12 & -100 & 600 & 600 & -100 & 12 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \end{bmatrix}.$$

For $k = 8$, the generator for the interior scheme of the gradient interpolator $I_G^{(8)}$ is $g_8 = [-\frac{7}{2}, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}]$. The generator associated to the interpolation near the boundary are $g_{81} = [-\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}, \frac{15}{2}]$, and $g_{82} = [-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}]$, and

$g_{83} = [-\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}]$. Thus, the non-zero entries of $I_G^{(8)}$ are given by

$$I_G^{(8)} = \begin{bmatrix} 1 & & & & & & & & \\ \frac{6435}{32768} & \frac{6435}{4096} & -\frac{15015}{8192} & \frac{9009}{4096} & -\frac{32175}{16384} & \frac{5005}{4096} & -\frac{4095}{8192} & \frac{495}{4096} & -\frac{429}{32768} \\ -\frac{429}{32768} & \frac{1287}{4096} & \frac{9009}{8192} & -\frac{3003}{4096} & \frac{9009}{16384} & -\frac{1287}{4096} & \frac{1001}{8192} & -\frac{117}{4096} & \frac{99}{32768} \\ \frac{99}{32768} & -\frac{165}{4096} & \frac{3465}{8192} & \frac{3465}{4096} & -\frac{5775}{16384} & \frac{693}{4096} & -\frac{495}{8192} & \frac{55}{4096} & -\frac{45}{32768} \\ -\frac{5}{2048} & \frac{49}{2048} & -\frac{245}{2048} & \frac{1225}{2048} & \frac{1225}{2048} & -\frac{245}{2048} & \frac{49}{2048} & -\frac{5}{2048} & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

7.2.1 The 2D and 3D gradient interpolation operators

For a Cartesian grid with m, n, o cells in the x, y, z-axes, respectively, they are constructed by utilizing the Kronecker product $\otimes$.

The 2D gradient interpolation operators $(I_G)_{xy}^{(k)}$ of k-th order are given by

$$(I_G)_{xy}^{(k)} = \begin{bmatrix} (I_G)_{xy,1}^{(k)} & \\ & (I_G)_{xy,2}^{(k)} \end{bmatrix} = \begin{bmatrix} \hat{I}_n \otimes (I_G)_x^{(k)} & \\ & (I_G)_y^{(k)} \otimes \hat{I}_m \end{bmatrix},$$

and the 3D gradient interpolation operators $(I_G)_{xyz}^{(k)}$ of k-th order are given by

$$\begin{aligned} (I_G)_{xyz}^{(k)} &= \begin{bmatrix} (I_G)_{xyz,1}^{(k)} & & \\ & (I_G)_{xy,2}^{(k)} & \\ & & (I_G)_{xyz,3}^{(k)} \end{bmatrix} \\ &= \begin{bmatrix} \hat{I}_o \otimes \hat{I}_n \otimes (I_G)_x^{(k)} & & \\ & \hat{I}_o \otimes (I_G)_y^{(k)} \otimes \hat{I}_m & \\ & & (I_G)_z^{(k)} \otimes \hat{I}_n \otimes \hat{I}_m \end{bmatrix}, \end{aligned}$$

where $(I_G)_p^{(k)}$ is the 1D divergence interpolation operator along the p-axis, and

$$\hat{I}_q = \begin{bmatrix} 0_{1\times q} \\ I_{q\times q} \\ 0_{1\times q} \end{bmatrix},$$

with $I_{q\times q}$ is the $q \times q$ identity matrix.

Notice that (9) implies

$$(I_G)_{xyz}\mathbb{1} = \mathbb{1}.$$

8 The quadrature weight operators

The 1D quadrature weight operators are constructed to satisfy the extended Gauss divergence theorem

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

In 1D, for $U = [a, b]$, this formula becomes the integration by parts formula (IBP)

$$\int_a^b v \, f' \, dx + \int_a^b f \, v' \, dx = f(b) \, v(b) - f(a) \, v(a).$$

If V is a discrete version of the 1D vector field v, with

$$\vec{V} = (V_0, V_1, \cdots, V_N)^T, \qquad V_j = v(x_j), \, x_j = a + jh, \qquad j = 0, 1, \cdots, N,$$

and F is a discrete version of the 1D scalar field f, with

$$F = (F_0, F_1, \cdots, F_{N+1})^T,$$

and

$$F_0 = f(a), \quad F_{N+1} = f(b), \quad F_j = f(x_j), \quad x_j = a + \frac{(2j-1)h}{2}, \quad j = 1, \cdots, N,$$

then the Corbino-Castillo mimetic discrete analog of the IBP formula is given by

$$h \, \langle GF, V \rangle_P + h \, \langle DV, F \rangle_Q = F_{N+1} V_N - F_0 V_0, \tag{11}$$

where D and G are the divergence and gradient operators, and where Q and P are convenient diagonal positive-definite square matrices called the quadrature weight operators for the divergence and the gradient, respectively.

8.1 The 1D divergence quadrature weight operators

The Corbino-Castillo 1D divergence quadrature weight operators Q are square matrices of order $(N+2) \times (N+2)$.

If in (11), one assumes the constant discrete scalar field $F = \mathbb{1} \in \mathbb{R}^{N+2}$, then (3) implies

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

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

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

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

$$h\, D^T Q\mathbb{1} = b_{N+1}^T. \tag{12}$$

If $q = (Q_{1,1}, \cdots, Q_{N+2,N+2}) = Q\mathbb{1}$ then system (12) can be rewritten as

$$h\, qD = b_{N+1},$$

which is a system of $N+1$ equations with $N+2$ unknowns. However, since the first and last rows of D are zero, $Q_{1,1}$ and $Q_{N+2,N+2}$ are not present in any of the $N+1$ equations, and they can be arbitrarily set to

$$Q_{1,1} = 1 = Q_{N+2,N+2}.$$

Hence, (12) reduces to a system of $N+1$ equations and N unknowns.

Observe that symmetry of D with respect to the center of interval $[a, b]$ imposes

$$Q_{N+3-i,N+3-i} = Q_{i,i}, \qquad i = 1, \ldots, N+2.$$

Therefore, one only needs to specify the first $\lceil \frac{N}{2} \rceil + 1$ entries.

For $k = 2$, it is easy to verify that due to $D^{(2)}$ weights $-1, 1$ for the interior cell centers, one has

$$Q^{(2)} = \text{diag}\ \{1, \cdots, 1\}.$$

Unfortunately, for $k = 4, 6, 8$, the diagonal entries of Q depend on the number of cells N and one observes that the weights approach a constant value around $Q_{\frac{N}{2}+1,\frac{N}{2}+1}$, value which is close to one. [2] As examples, consider

$$\begin{aligned}
Q^{(4)}_{N=9} &= \text{diag}\left\{1, \frac{157491}{139984}, \frac{52593}{69992}, \frac{162675}{139984}, \frac{648}{673}, \frac{8724}{8749}, \frac{648}{673}, \cdots\right\} \\
Q^{(4)}_{N=10} &= \text{diag}\left\{1, \frac{454949}{404376}, \frac{151927}{202188}, \frac{469925}{404376}, \frac{16224}{16849}, \frac{16824}{16849}, \frac{16824}{16849}, \cdots\right\} \\
Q^{(4)}_{N=11} &= \text{diag}\left\{1, \frac{12266099}{10902576}, \frac{4096177}{5451288}, \frac{12669875}{10902576}, \frac{218712}{227137}, \frac{226812}{227137}, \frac{227112}{227137}, \frac{226812}{227137}, \cdots\right\}
\end{aligned}$$

In Figure 2, one can see how $Q^{(4)}_{\lceil N/2\rceil+1,\lceil N/2\rceil+1}$ (the middle entry of $Q^{(4)}$) approaches 1 as the number of cells increases.

[2] In [5] page 6, it is established that the diagonal of Q is given by

$$\left[1, \frac{2186}{1943}, \frac{1992}{2651}, \frac{1993}{1715}, \frac{649}{674}, \frac{699}{700}, \frac{18170}{18171}, \frac{471744}{471745}, 1, \cdots\right].$$

These numbers where obtained inverting in MATLAB the D^T operator. A more precise approach is by computing the same algorithm with MAPLE. These numbers are utilized in the calculation of energy conservation and their differences in practical terms are negligible.

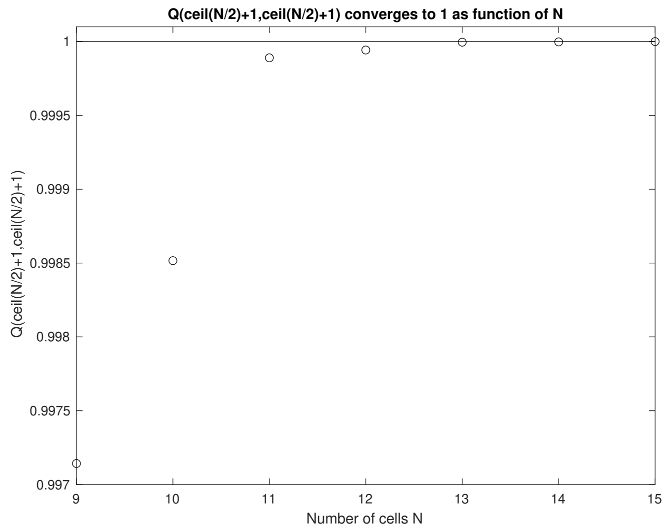

Figure 2: Q center divergence weight converges to 1 as the number of cells increases.

8.2 The 2D and 3D divergence quadrature weight operators

For a Cartesian grid with m, n, o cells in the x, y, z-axes, respectively, they are constructed by utilizing the Kronecker product $\otimes$.

The 2D divergence quadrature weight operator $\mathcal{Q}_{xy}^{(k)}$ of k-h order are given by

$$\mathcal{Q}_{xy}^{(k)} = \begin{bmatrix} I_{n+2} \otimes Q_{m+2}^{(k)} & \\ & Q_{n+2}^{(k)} \otimes I_{m+2} \end{bmatrix},$$

and the 3D divergence quadrature weight operator $\mathcal{Q}_{xyz}^{(k)}$ of k-h order are given by

$$\mathcal{Q}_{xyz}^{(k)} = \begin{bmatrix} I_{o+2} \otimes I_{n+2} \otimes Q_{m+2}^{(k)} & & \\ & I_{o+2} \otimes Q_{n+2}^{(k)} \otimes I_{m+2} & \\ & & Q_{o+2}^{(k)} \otimes I_{n+2} \otimes I_{m+2} \end{bmatrix},$$

where I_q is the $q \times q$ identity matrix.

8.3 The 1D quadrature gradient weight operators

The Corbino-Castillo 1D quadrature gradient weight operators P are diagonal positive-definite matrices of order $(N+1) \times (N+1)$.

If in (11), one assumes the constant discrete vector field $V = \mathbb{1} \in \mathbb{R}^{N+1}$, then (1) implies

$$h \langle GF, \mathbb{1} \rangle_P = F_{N+1} - F_0,$$

and, since $\langle GF, \mathbb{1}\rangle_P = \langle PGF, \mathbb{1}\rangle = \langle F, G^T P\mathbb{1}\rangle = F^T G^T P\mathbb{1}$, then

$$h\, F^T G^T P\mathbb{1} = F^T(-1, 0, \cdots, 0, 1)^T,$$

or equivalently, if $b_{N+2} = (-1, 0, \cdots, 0, 1) \in \mathbb{R}^{N+2}$ then

$$h\, G^T P\mathbb{1} = b^T_{N+2}. \tag{13}$$

Symmetry with respect to the center of interval $[a, b]$ imposes

$$P_{N+2-i,N+2-i} = P_{i,i}, \qquad i = 1, \ldots, N+1.$$

Therefore, one only needs to specify the first $\lceil \frac{N+1}{2} \rceil$ entries.

If $p_w = (P_{1,1}, \cdots, P_{N+1,N+1})^T$ then (13) becomes $G^T p = b^T_{N+2}$ which is a system of $N+2$ equations with $N+1$ unknowns.

For $k = 2$, it is easy to verify that due to $G^{(2)}$ weights $-1, 1$ for the interior cell faces, one has

$$P^{(2)} = \text{diag}\ \left\{\frac{3}{8}, \frac{9}{8}, 1, \cdots, 1, \frac{9}{8}, \frac{3}{8}\right\}$$

Unfortunately, for $k = 4, 6, 8$, the diagonal entries of P depend on the number of cells N and one observes that the weights approach a constant value around $P_{\frac{N}{2}+1,\frac{N}{2}+1}$, value which is close to one. [3] As examples, consider

$$\begin{aligned}
P^{(4)}_{N=8} &= \text{diag}\left\{\frac{297439}{839904}, \frac{257947}{209976}, \frac{754333}{839904}, \frac{1371}{1346}, \frac{17523}{17498}, \frac{1371}{1346} \cdots\right\}\\
P^{(4)}_{N=9} &= \text{diag}\left\{\frac{95469}{269584}, \frac{331173}{269584}, \frac{121059}{134792}, \frac{34323}{33698}, \frac{33723}{33698}, \frac{33723}{33698} \cdots\right\}\\
P^{(4)}_{N=10} &= \text{diag}\left\{\frac{7721957}{21805152}, \frac{3348343}{2725644}, \frac{19583579}{21805152}, \frac{462699}{454274}, \frac{454599}{454274}, \frac{454299}{454274}, \frac{454599}{454274} \cdots\right\}
\end{aligned}$$

In Figure 3, one can see how $P^{(4)}_{\lfloor N/2\rfloor+1,\lfloor N/2\rfloor+1}$ (the middle entry of $P^{(4)}$) approaches 1 as the number of cells increases.

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[3] In [5] page 6, it is established that the diagonal of P is given by

$$\left[\frac{227}{641}, \frac{941}{766}, \frac{811}{903}, \frac{1373}{1348}, \frac{1401}{1400}, \frac{36343}{36342}, \frac{943491}{943490}, 1, \cdots\right].$$

These numbers where obtained inverting in MATLAB the G^T operator. A more precise approach is by computing the same algorithm with MAPLE. These numbers are utilized in the calculation of energy conservation and their differences in practical terms are negligible.

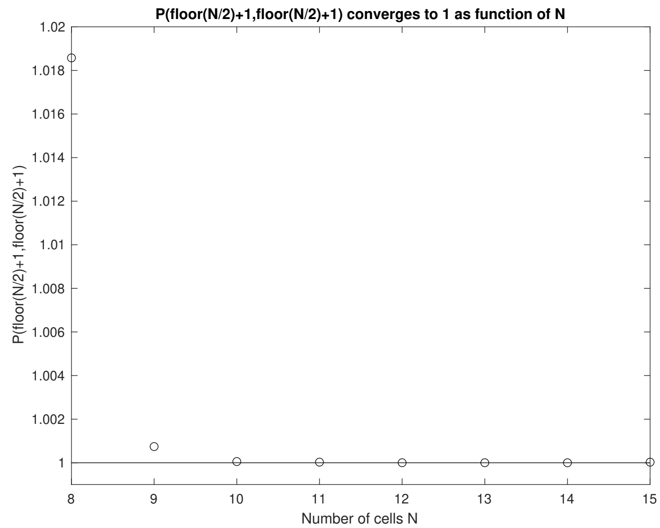

Figure 3: P center divergence weight converges to 1 as the number of cells increases.

8.4 The 2D and 3D gradient quadrature weight operators

For a Cartesian grid with m, n, o cells in the x, y, z-axes, respectively, they are constructed by utilizing the Kronecker product $\otimes$.

The 2D gradient quadrature weight operator $\mathcal{P}_{xy}^{(k)}$ of k-h order are given by

$$\mathcal{P}_{xy}^{(k)} = \begin{bmatrix} I_{n+2} \otimes P_{m+2}^{(k)} & \\ & P_{n+2}^{(k)} \otimes I_{m+2} \end{bmatrix},$$

and the 3D gradient quadrature weight operator $\mathcal{P}_{xyz}^{(k)}$ of k-h order are given by

$$\mathcal{P}_{xyz}^{(k)} = \begin{bmatrix} I_{o+2} \otimes I_{n+2} \otimes P_{m+2}^{(k)} & & \\ & I_{o+2} \otimes P_{n+2}^{(k)} \otimes I_{m+2} & \\ & & P_{o+2}^{(k)} \otimes I_{n+2} \otimes I_{m+2} \end{bmatrix},$$

where I_q is the $q \times q$ identity matrix.

9 The 1D Boundary operators

Equation (11) can be written as

$$h \langle F, G^T PV \rangle + h \langle F, QDV \rangle = F_{N+1}V_N - F_0V_0,$$

and hence if one defines

$$B = h\,(QD + G^T P) \in \mathbb{R}^{(N+2)\times(N+1)},$$

and $\bar{B} \in \mathbb{R}^{(N+2)\times(N+1)}$ by

$$\bar{B} = \begin{pmatrix} -1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix},$$

then (11) becomes

$$F^T B V = F^T \bar{B} V.$$

In addition, for $1 \le i \le N+2$, the corresponding row sums of B are

$$\begin{aligned} \sum_{j=1}^{N+1} B_{ij} &= h \sum_{j=1}^{N+1} (G^T P + QD)_{ij} = h \sum_{j=1}^{N+1} \sum_{l=1}^{N+2} (G^T_{il} P_{lj} + Q_{il} D_{lj}) \\ &= h \sum_{j=1}^{N+1} \sum_{l=1}^{N+2} (G^T_{il}\, p_l\, \delta_{lj} + q_i\, \delta_{il}\, D_{lj}) = h \sum_{j=1}^{N+1} G^T_{ij} p_j + h\, q_i \sum_{j=1}^{N+1} D_{ij} \\ &= h\, G^T_{i\cdot} P \mathbb{1} = \begin{cases} -1, & i = 1, \\ 0, & 2 \le i \le N+1, \\ 1, & i = N+2 \end{cases} \end{aligned}$$

where δ_{ij} is the Kronecker delta. The last identity follows from (13) and (1).

All row sums of $E = B - \bar{B}$ are zero. So, E is of order h, and $E \to 0$ as $h \to 0$.

Because of the sizes of matrices $D_{xyz}, \mathcal{Q}_{xyz}, G_{xyz}, \mathcal{P}_{xyz}$, and since (11) can be written as

$$h\,\langle V, PGF\rangle + h\,\langle V, Q_{N+1} D^T F\rangle = F_{N+1} V_N - F_0 V_0,$$

where Q_{N+1} is the Q matrix of order $(N+1)\times(N+1)$ instead of order $(N+2)\times(N+2)$, then the 3D version of the boundary operators are defined by

$$B_{xyz} = h_x h_y h_z\, \mathcal{P}_{xyz} G_{xyz} + h_x h_y h_z\, \mathcal{Q}_{3(m+1)(n+1)(o+1),xyz} D^T_{xyz},$$

where $\mathcal{Q}_{3(m+1)(n+1)(o+1),xyz}$ has order $3(m+1)(n+1)(o+1) \times 3(m+1)(n+1)(o+1)$, and

$$\bar{B}_{xyz} = \begin{pmatrix} I_{o+2} \otimes I_{n+2} \otimes \bar{B}_x & & \\ & I_{o+2} \otimes \bar{B}_y \otimes I_{m+2} & \\ & & \bar{B}_z \otimes I_{n+2} \otimes I_{m+2} \end{pmatrix},$$

where $\bar{B}_p$ is the one dimensional boundary $\bar{B}$ matrix along the p-axis.

10 The extended Gauss divergence theorem

The extended Gauss divergence theorem is given by

$$\int_U \vec{v} \cdot \nabla f \; dU + \int_U f \, \nabla \cdot \vec{v} \; dU = \int_{\partial U} f \, \vec{v} \cdot \vec{n} \; dS$$

By construction, see (11), its Corbino-Castillo mimetic analog in 1D (or IBP formula) is given by

$$h\big\langle DV, F\big\rangle_Q + h\big\langle V, GF\big\rangle_P = F_{N+1}V_N - F_0V_0.$$

The generalization of the IBP formula to the 3D extended Gauss divergence theorem is

$$\vec{V} B_{xyz} F = \vec{V} \bar{B}_{xyz} F, \tag{14}$$

where $\vec{V} = (V_1, V_2, V_3)$ is the discrete version of the 3D vector field $\vec{v} = (v_1, v_2, v_3)$ and F is the discrete version of the scalar field f.

Therefore, one gets

$$h_x h_y h_z \, \langle \mathcal{P}_{xyz} G_{xyz} F, \vec{V} \rangle + h_x h_y h_z \, \langle \mathcal{Q}_{3(m+1)(n+1)(o+1),xyz} D^T_{xyz} F, \vec{V} \rangle = F^T \bar{B}_{xyz} \vec{V}.$$

If $F \equiv \mathbb{1}$, then

$$h_x h_y h_z \, \mathbb{1}^T D_{xyz} \mathcal{Q}_{3(m+1)(n+1)(o+1),xyz} \vec{V} = \mathbb{1}^T \bar{B}_{xyz} \vec{V}.$$

Since, it is valid for all $\vec{V}$ then

$$h_x h_y h_z \, \mathbb{1}^T D_{xyz} \mathcal{Q}_{3(m+1)(n+1)(o+1),xyz} = \mathbb{1}^T \bar{B}_{xyz},$$

and

$$h_x h_y h_z \, \mathcal{Q}_{3(m+1)(n+1)(o+1),xyz} D^T_{xyz} \mathbb{1} = \bar{B}^T_{xyz} \mathbb{1} = \begin{pmatrix} \mathbb{1} \otimes \mathbb{1} \otimes b_{m+1} & & \\ & \mathbb{1} \otimes b_{n+1} \otimes \mathbb{1} & \\ & & b_{o+1} \otimes \mathbb{1} \otimes \mathbb{1} \end{pmatrix}. \tag{15}$$

Similarly, since

$$h_x h_y h_z \, \langle F, G^T_{xyz} \mathcal{P}_{xyz} \vec{V} \rangle + h_x h_y h_z \, \langle F, \mathcal{Q}_{xyz} D_{xyz} \vec{V} \rangle = F^T \bar{B}_{xyz} \vec{V}.$$

If $\vec{V} = \mathbb{1}$, then

$$h_x h_y h_z \, F^T G^T_{xyz} \mathcal{P}_{xyz} \mathbb{1} = F^T \bar{B}_{xyz} \mathbb{1}.$$

Since, it is valid for all F, then

$$h_x h_y h_z \, G^T_{xyz} \mathcal{P}_{xyz} \mathbb{1} = \bar{B}_{xyz} \mathbb{1} = \begin{pmatrix} \mathbb{1} \otimes \mathbb{1} \otimes b_{m+2} & & \\ & \mathbb{1} \otimes b_{n+2} \otimes \mathbb{1} & \\ & & b_{o+2} \otimes \mathbb{1} \otimes \mathbb{1} \end{pmatrix}. \tag{16}$$

11 Some Vector Calculus Identities

In this section, Corbino-Castillo mimetic discrete analogs of some of the vector calculus identities are derived.

Given scalars α, β, the 3D scalar fields f, g and the 3D vector fields $\vec{v}, \vec{w}$, the discrete analogs of the scalar fields are

$$F, G : S^1 \times S^2 \times S^3 \to \mathbb{R},$$

and the discrete analogs of the vector fields are $\vec{V}, \vec{W}$ with $\vec{V} = (V_1, V_2, V_3), \vec{W} = (W_1, W_2, W_3)$, where

$$V_1, W_1 : N^1 \times S^2 \times S^3 \to \mathbb{R}, \qquad V_2, W_2 : S^1 \times N^2 \times S^3 \to \mathbb{R}, \qquad V_3, W_3 : S^1 \times S^2 \times N^3 \to \mathbb{R}.$$

Discrete analogs of some vector calculus identities are found while trying to remove the dependence on discrete versions of scalar and vector fields.

The list of vector calculus identities is the following.

1. The linearity of the divergence, or

$$\nabla \cdot (\alpha\, \vec{v} + \beta \vec{w}) = \alpha\, \nabla \cdot \vec{v} + \beta\, \nabla \cdot \vec{w}.$$

   It follows from the matrix representation of the divergence mimetic operators.

$$D_{xyz}(\alpha\, \mathrm{vec}_L(\vec{V}) + \beta\, \mathrm{vec}_L(\vec{W})) = \alpha\, D_{xyz}\, \mathrm{vec}_L(\vec{V}) + \beta\, D_{xyz}\, \mathrm{vec}_L(\vec{W}).$$

   where

$$\mathrm{vec}(\vec{U})_L = \, (\mathrm{vec}_L(U_1), \mathrm{vec}_L(U_2), \mathrm{vec}_L(U_3))^T,$$

   with $\mathrm{vec}_L(T)$ the vectorization operator in lexicographic order of the discrete vector field component T.

2. The linearity of the gradient, or

$$\nabla(\alpha\, f + \beta g) = \alpha\, \nabla f + \beta\, \nabla g.$$

   It follows from the matrix representation of the gradient mimetic operators.

$$G_{xyz}(\alpha\, \mathrm{vec}_L(F) + \beta\, \mathrm{vec}_L(G)) = \alpha\, G_{xyz}\, \mathrm{vec}_L(F) + \beta\, G_{xyz}\, \mathrm{vec}_L(G).$$

   with $\mathrm{vec}_L(H)$ the vectorization operator in lexicographic order of the discrete scalar field H.

3. The divergence of a constant vector field: for a 3D constant vector field $\vec{v} = a\vec{i}+b\vec{j}+c\vec{k}$, with a, b, c real constants, one has

$$\nabla \cdot \vec{v} = 0.$$

The discrete analog

$$D_{xyz}(a\,\hat{I}_o^T \otimes \hat{I}_n^T \otimes \mathbb{1}_{m+2} + b\,\hat{I}_o^T \otimes \mathbb{1}_{n+2} \otimes \hat{I}_m^T + c\,\mathbb{1}_{o+2} \otimes \hat{I}_n^T \otimes \hat{I}_m^T) = 0,$$

follows from the definition of D_{xyz} by Kronecker products and (1).

4. The gradient of a constant scalar field, or

$$\nabla\, 1 = \vec{0}.$$

The discrete analog

$$G_{xyz}\mathbb{1}_{(m+2)(n+2)(o+2)} = 0,$$

follows from the definition of G_{xyz} by Kronecker products and (3).

5. The Laplacian, or

$$\Delta f = \nabla \cdot \nabla f.$$

It follows from the definition of Laplacian mimetic operators that

$$L_{xyz}F = D_{xyz}G_{xyz}F.$$

6. The gradient of a product of a product of scalar fields:

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

If one integrates this identity over the domain, one gets

$$\int_U \nabla(fg)\,dU = \int_U f\,\nabla g\,dU + \int_U g\,\nabla f\,dU.$$

The mimetic discrete analog of this identity is

$$\langle G_{xyz}(\mathrm{diag}(f))g, \mathbb{1}\rangle_{\mathcal{P}_{xyz}} = \langle G_{xyz}g, (I_D)_{xyz}f\rangle_{\mathcal{P}_{xyz}} + \langle G_{xyz}f, (I_D)_{xyz}g\rangle_{\mathcal{P}_{xyz}},$$

where, to simplify notation f, g are the discrete versions of f, g.

The previous identity can be written as

$$g^T \mathrm{diag}(f)G_{xyz}^T\mathcal{P}_{xyz}\mathbb{1} = g^T G_{xyz}^T P(I_D)_{xyz}f + g^T(I_D)_{xyz}^T\mathcal{P}_{xyz}G_{xyz}f.$$

Since, it is valid for any g then

$$\mathrm{diag}(f)G_{xyz}^T\mathcal{P}_{xyz}\mathbb{1} = G_{xyz}^T\mathcal{P}_{xyz}(I_D)_{xyz}f + (I_D)_{xyz}^T\mathcal{P}_{xyz}G_{xyz}f.$$

Multiply on the left by $(\mathbb{1})^T$ one gets

$$\begin{aligned}(\mathbb{1})^T \mathrm{diag}(f) G_{xyz}^T \mathcal{P}_{xyz} \mathbb{1} &= (\mathbb{1})^T G_{xyz}^T \mathcal{P}_{xyz} (I_D)_{xyz} f + (\mathbb{1})^T (I_D)_{xyz}^T \mathcal{P}_{xyz} G_{xyz} f \\ (\mathbb{1})^T \mathcal{P}_{xyz} G_{xyz} f = f^T G_{xyz}^T \mathcal{P}_{xyz} \mathbb{1} &= (G_{xyz}\mathbb{1})^T \mathcal{P}_{xyz} (I_D)_{xyz} f + ((I_D)_{xyz}\mathbb{1})^T \mathcal{P}_{xyz} G_{xyz} f.\end{aligned}$$

Since the last identity is valid for any f then

$$(\mathbb{1})^T \mathcal{P}_{xyz} G_{xyz} = (G_{xyz}\mathbb{1})^T \mathcal{P}_{xyz} (I_D)_{xyz} + ((I_D)_{xyz}\mathbb{1})^T \mathcal{P}_{xyz} G_{xyz}.$$

The first term of the right hand side is zero because of (5). The identity follows from (8).

One can show that the differential version of this identity actually holds in 1D, if the gradient interpolation operator is of order two. For, consider the mimetic analog

$$G(f \circ g) = I_D f \circ Gg + I_D g \circ Gf,$$

where $\circ$ is the component-wise or Hadamard product.

For the boundary points the data to be interpolated is known and hence the first row of (I_D) is $(1, 0, \cdots, 0)$ and its last row is $(0, \cdots, 0, 1)$.

For the other rows of I_D consider the following. If $1 < i < N+1$, the i-th component of the previous identity is given by

$$\sum_{k=1}^{N+2} G_{ik} f_k g_k = \left(\sum_{l=1}^{N+2} (I_D)_{il} f_l\right)\left(\sum_{k=1}^{N+2} G_{ik} g_k\right) + \left(\sum_{l=1}^{N+2} (I_D)_{ik} g_k\right)\left(\sum_{l=1}^{N+2} G_{il} f_l\right).$$

Or, equivalently,

$$\sum_{k=1}^{N+2}\sum_{l=1}^{N+2} G_{ik}\delta_{kl} g_k f_l = \sum_{k=1}^{N+2}\sum_{l=1}^{N+2} ((I_D)_{il} G_{ik} + (I_D)_{ik} G_{il}) f_l g_k.$$

Since the last identity is valid for any f, g, then

$$G_{ik}\delta_{kl} = (I_D)_{il} G_{ik} + (I_D)_{ik} G_{il}.$$

If $G_{ik} = 0$, then set $(I_D)_{ik} = 0$. So, I_D is zero wherever G is zero.

It is known that for $1 < i < N+1$, one has $G_{i,i} = -1, G_{i,i+1} = 1$ and $G_{i,k} = 0$ for $k \neq i, i+1$. If $k = i$, then $-\delta_{il} = -(I_D)_{il} + (I_D)_{ii} G_{il}$. If, in addition, $l = i$ then $(I_D)_{i,i} = \frac{1}{2}$. If, instead $l = i+1$, then $(I_D)_{i,i+1} = (I_D)_{i,i} = \frac{1}{2}$.

This is the divergence interpolation operator I_D of order two.

7. The product rule for a multiplication by a scalar of the divergence: for a 3D scalar field f and a 3D vector field $\vec{v}$, one has

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

If one integrates this identity over the domain, one gets

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

The extended Gauss divergence theorem implies that

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

and for $\vec{w} = f\,\vec{v}$, one has

$$\int_U \nabla \cdot \vec{w}\,dU = \int_{\partial U} \vec{w} \cdot \vec{n}\,dS.$$

The mimetic analog reads, for the discrete version $\vec{W}$ of vector field $\vec{w}$,

$$\langle D_{xyz}\vec{W}, \mathbb{1}\rangle_{\mathcal{Q}_{xyz}} = \vec{V} B_{xyz} F = \vec{V} \bar{B}_{xyz} F,$$

which is the 3D analog of the extended Gauss divergence theorem.

8. The Laplacian of a product of scalar fields:

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

If one integrates this identity over the domain, one gets

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

The mimetic analog is

$$\langle D_{xyz}G_{xyz}(f \circ g), \mathbb{1}\rangle_{\mathcal{Q}_{xyz}} = \langle D_{xyz}G_{xyz}g, f\rangle_{\mathcal{Q}_{xyz}} + 2\,\langle (I_G)_{xyz}g, (I_G)_{xyz}f\rangle_{\mathcal{Q}_{xyz}} + \langle D_{xyz}G_{xyz}f, g\rangle_{\mathcal{Q}_{xyz}},$$

or, equivalently,

$$g^T(\mathrm{diag}(f))G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz}\mathbb{1} = g^T G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz} f + 2\,g^T G_{xyz}^T (I_G)_{xyz}^T \mathcal{Q}_{xyz} (I_G)_{xyz} G_{xyz} f + g^T \mathcal{Q}_{xyz} D_{xyz} G_{xyz} f.$$

Since the last identity is valid for all g, one has

$$(\mathrm{diag}(f))G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz}\mathbb{1} = G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz} f + 2\,G_{xyz}^T (I_G)_{xyz}^T \mathcal{Q}_{xyz} (I_G)_{xyz} G_{xyz} f + \mathcal{Q}_{xyz} D_{xyz} G_{xyz} f.$$

Multiplying on the left by $\mathbb{1}^T$, and since

$$\mathbb{1}^T(\mathrm{diag}(f))G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz}\mathbb{1} = f^T G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz}\mathbb{1} = \mathbb{1}^T \mathcal{Q}_{xyz} D_{xyz} G_{xyz} f,$$

then

$$\mathbb{1}^T \mathcal{Q}_{xyz} D_{xyz} G_{xyz} f = \mathbb{1}^T G_{xyz}^T D_{xyz}^T \mathcal{Q}_{xyz} f + 2\,\mathbb{1}^T G_{xyz}^T (I_G)_{xyz}^T \mathcal{Q}_{xyz} (I_G)_{xyz} G_{xyz} f + \mathbb{1}^T \mathcal{Q}_{xyz} D_{xyz} G_{xyz} f.$$

The last identity is valid for any f. It follows that

$$\mathbb{1}^T \mathcal{Q}_{xyz} D_{xyz} G_{xyz} = (G_{xyz}\mathbb{1})^T D_{xyz}^T \mathcal{Q}_{xyz} + 2\,(G_{xyz}\mathbb{1})^T (I_G)_{xyz}^T \mathcal{Q}_{xyz} (I_G)_{xyz} G_{xyz} + \mathbb{1}^T \mathcal{Q}_{xyz} D_{xyz} G_{xyz}.$$

The first two terms of the right hand side are zero because of (5). The identity follows.

12 Conclusions and future work

The purpose of this document is to demonstrate in what sense mimetic differences operators satisfy a discrete analog of some 3D vector calculus formulas. Even though these proofs are shown for the Corbino-Castillo mimetic differences, the same approach applies for the Castillo-Grone mimetic differences since no particular feature of the Corbino-Castillo method is utilized.

A high-order discrete analog of the 1D integration by parts formula is central in any of the mimetic difference methods. Indeed, this property causes the fact that high-order discrete analogs of some vector calculus identities are valid in the integral sense. Nevertheless, it is also exhibited that some vector calculus identities, in the differential sense, can be established if one gives up on high-order accuracy.

When establishing discrete analogs of these identities, one needs to use 3D interpolation operators, as well as 3D extensions of weight matrices P and Q, boundary matrices and some other identities that derive from the 3D integration by parts formula (or extended Gauss divergence theorem). Since, these extensions can be found widespread in references or are not published at all, they are collected here. Moreover, the derivation of the Corbino-Castillo mimetic operators provided in this work avoids inverting explicitly Vandermonde matrices.

One of our future immediate extensions of mimetic differences operators is to develop a matrix representation of the curl operator that satisfies discrete analogs of some vector calculus properties. This will facilitate applications of mimetic methods in electromagnetism, as well as in other areas.

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