

Research Article

High Order Mimetic Finite Difference Operators Satisfying a Gauss Divergence Theorem

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Abstract

High order mimetic finite difference operators that satisfy a discrete extended Gauss Divergence theorem are presented. These operators have the same order of accuracy in the interior as well as the boundary, no free parameters and optimal bandwidth. They are constructed on staggered grids, using weighted inner products with a diagonal norm. We present several examples to demonstrate that mimetic finite difference schemes using these operators produce excellent results.

Keywords: Mimetic; Finite-difference; Castillo-Grone method; Differential operators; High-order

AMS subject classifications: 65D25, 65M06, 65N06

Introduction

Mimetic finite differences method have been experiencing a great deal of development in the last 10 years [1-5] and many applications of these methods have been reported in the literature. High order mimetic finite differences can be traced back to the work of Kreiss and Scherer [1], where they presented the Summation by Parts method (SBP). From their work, it is known that the order of accuracy at the boundary cannot be increased, with standard inner products, on nodal grids. They constructed a high order SBP operator, increasing the order of accuracy at the boundary [6-15], with a weighted inner product, on nodal grids. This operator was two orders less accurate at the boundary than the interior of the domain, on a nodal grid, with a diagonal weight matrix norm. In 2003, Castillo and Grone [7] using weighted inner products and staggered grids, constructed high-order divergence and gradient mimetic finite differences operators with the same order of accuracy in the interior as well as the boundary. These operators (CG) have been extended to higher dimensions and have been used very successfully in several applications [16-25]. However, these discrete operators have a set of free parameters and not necessarily the optimum bandwidth. In this paper, we construct high-order mimetic finite differences operators' divergence and gradient, on staggered grids, with diagonal weight matrix norms, no free parameters and optimal bandwidth. Some examples comparing the CG operators with the ones presented, exhibit results clearly showing that the new operators produce better results than that of the CG ones and in the worst case they produce the same ones.

This paper is organized as follows: We give a brief description of mimetic operators along with their properties, and the staggered grids along with a 3-D cell for illustration. We show how to construct the one dimensional second order mimetic gradient operator and show the gradient and divergence for the fourth order case. Note that for the second order case these operators are the same as the CG ones, but this only happens for the second order case, for fourth order and higher the new operators are different from the CG ones. We describe how to compute the weights for the inner products for the fourth order gradient and divergence mimetic finite difference operators. We show how to construct the operators in higher dimensions using Kronecker products as well as a mimetic finite difference Laplacian in one, two and three dimensions as well and the mimetic finite difference curl operator.

We show how these operators can be implemented in a compact form, minimizing the size of the stencils. We present examples that clearly demonstrate the new operators produce better results that the CG ones.

Mimetic Operators

Mimetic finite difference operators, divergence (D), gradient (G), curl (C) and laplacian (L) are discrete analogs of their corresponding continuum operators. These mimetic finite difference operators satisfy in the discrete sense the vector identities that the continuum ones do making them more faithful to the physics.

Basic properties

Mimetic operators ($G \equiv \nabla$, $D \equiv \nabla$, $C \equiv \nabla \times$ and $L \equiv \nabla^2$) fulfill the following:

$$\mathbf{G}f_{const=}\mathbf{0},$$
 (1)

$$\mathbf{D}\mathbf{v}_{\text{courte}}\mathbf{0},$$
 (2)

$$\mathbf{CG} f=0,$$
 (3)

 $DC\nu=0,$ (4)

In addition, while providing a uniform order of accuracy, CG operators satisfy:

$$\langle \mathbf{D} v, f \rangle_{O_{+}} \langle \mathbf{G} f, v \rangle_{P} = \langle \mathbf{B} v, f \rangle$$
 (6)

which is a discrete analogue of the *extended Gauss divergence theorem* [8], here **B** is called the *mimetic boundary operator*. From eqn. (6) we obtain:

 $\langle Q\mathbf{D}\nu\rangle f + \langle P\mathbf{G}f,\nu\rangle = \langle \mathbf{B}\nu,f\rangle,$

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(7)

$$\langle \mathbf{Q}\mathbf{D}\mathbf{v} \rangle + \mathbf{G}^T P \mathbf{v} \cdot \mathbf{f} \rangle = \langle \mathbf{B}\mathbf{v}, \mathbf{f} \rangle,$$

 $\mathbf{Q}\mathbf{D}\mathbf{v} + \mathbf{G}^T P \mathbf{v} = \mathbf{B}\mathbf{v},$
 $\mathbf{Q}\mathbf{D} + \mathbf{G}^T P = \mathbf{B}.$

Staggered grids

CG mimetic operators are defined over staggered grids. In this type of grids, scalar variables are stored at the centers of the cells; while vector components are placed at the edges (or faces, in 3D). In the following figures, m, n and o represent the number of cells along the x-, y- and z-axes, respectively (Figures 1-4).

1D Operators

This section is focused on the construction of one-dimensional mimetic gradient and divergence operators. One-dimensional operators can be visualized as follows:

In Figure 5, A and A' are sub matrices that approximate the derivatives at the left, and at the right boundary, respectively. Dim(A)=Dim(A'), and A' is a permutation of A. M is a banded matrix of width k (order of accuracy) that approximates the derivatives at the









Figure 4: A 3D cell. u, v and w are the vector components used to compute the divergence. In case of the curl, we use the components that are tangential to the faces of the cell.



inner cells. The dimensions of *A* depend on the type of operator and the desired order of accuracy.

Gradient

To construct a *kth*-order mimetic gradient operator we need at least 2k cells ($m \ge 2k$) so that there is no overlapping between A and A'.

A and A' will have dimensions $\frac{k}{2}$ by k + 1. We proceed to construct a Vandermonde matrix from the stencil (Figure 6), then, our "generator" vector is:

$$\left[0\frac{1}{2}\frac{3}{2}\right] \tag{8}$$

and the corresponding Vandermonde matrix,

$$\begin{array}{c}
0 \ \frac{1}{4} \ \frac{9}{4} \\
0 \ \frac{1}{2} \ \frac{3}{2} \\
1 \ 1 \ 1 \ 1
\end{array}$$
(9).

Finally, we construct a right-hand side vector that only contains a '1' aligned to the second to last row of the matrix, producing the following system of linear equations:

$$\begin{bmatrix} 0 & \frac{1}{4} & \frac{9}{4} \\ 0 & \frac{1}{2} & \frac{3}{2} \\ 1 & 1 & 1 \\ \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$
(10)





and from the solution $[x_1, x_2, x_3] = \left[\frac{-8}{3} \cdot 3 \cdot \frac{-1}{3}\right]$, we obtain the first row of our matrix *A*. To obtain the successive rows of *A* we just need to "shift" the stencil to the right $\frac{k}{2}$ -1 time and is computed as follows:

$$A^{0=}-P_{p}AP_{q},$$
(11)

 $\frac{k}{2}$ where, P_p and P_q are permutation matrices with dimensions $\frac{k}{2}$ by and k+1 by k+1, respectively. To construct the sub matrix M we use a centered stencil (Figure 7), which produces the following system

$$\begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
(12)

and from the solution $[x_1, x_2] = [-1 \ 1]$, we obtain the rows of *M*. Putting all together we get:

$$G = \frac{1}{\Delta x} \begin{bmatrix} -\frac{8}{3} & 3 & -\frac{1}{3} \\ & -1 & 1 \\ & \ddots & \ddots \\ & & -1 & 1 \\ & & \frac{1}{3} & -3 & \frac{8}{3} \end{bmatrix}_{(m+1)(m+2)}$$
(13)

The 2^{nd} -order one-dimensional mimetic gradient. For higher orders, our resulting gradient operators differ from CG. Here we present our 4^{th} -order G:

$$G = \frac{1}{\Delta x} \begin{bmatrix} \frac{-352}{105} & \frac{35}{8} & \frac{-35}{24} & \frac{21}{40} & \frac{-5}{56} & 0 \dots \\ \frac{16}{105} & \frac{-31}{24} & \frac{29}{24} & \frac{-3}{40} & \frac{1}{168} & 0 \dots \\ 0 & \frac{1}{24} & \frac{-9}{8} & \frac{9}{8} & \frac{-1}{24} & 0 & \dots \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & \\ \vdots & 0 & \ddots & \ddots & \ddots & \ddots & \\ \end{bmatrix}_{(m+1)(m+2)}$$
(14)

In eqn. (14) we show only the set of rows necessary to illustrate the overall structure of the matrix.

Divergence

To construct a *kth*-order mimetic divergence operator we need at least 2k+1 cells ($m \ge 2k+1$) so that there is no overlapping between *A* and *A*'.

The methodology to construct a mimetic divergence is the same used to construct the mimetic gradient; except that A and A^0 will have dimensions $\frac{k}{2}$ -1 by k+1.As before, we first exhibit the 2nd-order operator.

Page 3 of 6

$$D = \frac{1}{\Delta x} \begin{bmatrix} 0 & \cdots & \\ -1 & 1 & \\ \ddots & \ddots & \\ & -1 & 1 & \\ & \dots & 0, \end{bmatrix}_{(m+2),(m+1)}$$
(15).

Notice that the first and last rows of eqn. (15) are zero, this is because on one hand, the divergence does not have a physical meaning at the boundary nodes, and on the other hand, formula in eqn. (6) needs D and G to me compatible matrices under addition, and G^{t} is (m+2) by (m+1), while D without "augmentation", is m by (m+1). Our resulting divergence operators differ from CG when $k \ge 4$. Here is our 4^{th} -order D:

$$D = \frac{1}{\Delta x} \begin{bmatrix} 0 & \cdots & & \\ \frac{-11}{12} & \frac{17}{24} & \frac{3}{8} & \frac{-5}{24} & \frac{1}{24} & 0 & \cdots \\ \frac{1}{24} & \frac{-9}{8} & \frac{9}{8} & \frac{-1}{24} & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \\ \end{bmatrix}_{(m+2),(m+1)}$$
(16)

again, in eqn. (16), we present only the set of rows necessary to illustrate the overall structure of the matrix.

Weight Matrix P

The diagonal weight matrix *P* (in eqn. (6)) is obtained by:

$$\mathbf{G}^{T} \boldsymbol{p} = \boldsymbol{b}_{m+2} \tag{17}$$

where *p* is the main diagonal of *P*, and b_{m+2} is the desired column sum $[-1 \cdots 0 \cdots 1]^T$.

For a 2nd-order **G**, the solution is
$$\frac{k}{2} p = \left[\frac{3}{8} \frac{9}{8} \dots 1 \dots \frac{9}{8} \frac{3}{8}\right]^T$$
. System in

eqn. (17) is over determined but consistent. For our 4th-order **G** (and m=20), we get:

$$p = \left[\frac{227}{641} \frac{941}{766} \frac{811}{903} \frac{1373}{1348} \frac{1401}{1400} \frac{36343}{36342} \frac{943491}{943490} 1 \dots \right]^{T}$$
(18)

Weight matrix Q

The same procedure is applied to get matrix *Q* (also from in eqn. (6),

$$\mathbf{D}^{T}q = b_{m+1}, \tag{19}$$

System in eqn. (19) is also overdetermined but consistent, and has solution $q = \vec{1}$ for a *2nd*-order **D**. In case of our *4th*-order **D** (and *m*=20), we get:

$$q = \left[1 \frac{2186}{1943} \frac{1992}{2651} \frac{1993}{1715} \frac{649}{674} \frac{699}{674} \frac{18170}{18171} \frac{471744}{471745} 1 \dots \right]^T$$
(20)

2D and 3D Operators

In this section we explain how to construct higher dimensional operators using the ones from and Kronecker products.

To construct a two-dimensional gradient:

$$G_{x,y} = \begin{bmatrix} S_x \\ S_y \end{bmatrix}$$
(21)

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where,

$$Sx = \hat{I}_n^T \otimes \mathbf{G}_x, \tag{22}$$

$$Sy = G_v \otimes \widehat{I}_m^T, \tag{23}$$

 \mathbf{G}_{x} , \mathbf{G}_{y} are the one-dimensional mimetic gradient operators for x and y, respectively. I_{m} denotes an "augmented" identity matrix (first and last rows are zero),

$$\hat{I}_{m} = \begin{bmatrix} 0 & \cdots \\ 1 \\ & \ddots \\ & 1 \\ & \cdots & 0 \end{bmatrix}_{(m+2),m}$$
(24)

To construct a three-dimensional gradient:

$$G_{x,y} = \begin{vmatrix} S_x \\ S_y \\ S_z \end{vmatrix}$$
(25)

where,

$$S_{x} = \widehat{I}_{o}^{T} \otimes \widehat{I}_{n}^{T} \otimes \mathbf{G}_{x}, \tag{26}$$

$$S_{y} = \widehat{I}_{o}^{T} \otimes \mathbf{G}_{y} \otimes \widehat{I}_{m}^{T},$$

$$S_{z} = G_{z} \otimes \widehat{I}_{n}^{T} \otimes \widehat{I}_{m}^{T}.$$
(27)
(27)
(28).

Here, $\mathbf{G}_x, \mathbf{G}_y, \mathbf{G}_z$ are the one-dimensional mimetic gradient operators for *x*, *y* and *z*, respectively.

To construct a two-dimensional divergence:

$$\mathbf{D}_{x,y} = [S_{x}, S_{y}] \tag{29}$$

where,

$$S_x = \hat{I}_n \otimes D_x, \tag{30}$$

$$S_{y} = D_{y} \otimes \widehat{I}_{n}, \tag{31}.$$

 \mathbf{D}_x , \mathbf{D}_y are the one-dimensional mimetic divergence operators for x and y, respectively.

To construct a three-dimensional divergence:

where,

$$D_{xyz} = [S_x, S_y, S_z],$$
 (32)

$$S_x = \hat{I}_0 \otimes \hat{I}_n \otimes D_x, \tag{33}$$

$$S_{y} = I_{0} \otimes D_{y} \otimes I_{m}, \tag{34}$$

$$S_z = D_z \otimes \tilde{I}_n \otimes \tilde{I}_m. \tag{35}$$

 $\mathbf{D}_{x}\mathbf{D}_{y}\mathbf{D}_{z}$ are the one-dimensional mimetic divergence operators for *x*, *y* and *z*, respectively.

One-, two- and three-dimensional laplacian operators are obtained by:

$$L_{x=}D_{x}G_{x},$$

$$Lxy=DxyGxy,$$
(36)
(37)

Lxyz=DxyzGxyz. (38)

Given a three-dimensional vector field:

 $\mathbf{F} = U\mathbf{i} + V \,\mathbf{j} + W\mathbf{k},\tag{39}$

the curl is defined as,

$$\Delta \times \mathbf{F} = \begin{vmatrix} i & j & k \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ U & V & W \end{vmatrix} = \left(\frac{\partial W}{\partial y} - \frac{\partial V}{\partial z}\right) i + \left(\frac{\partial U}{\partial z} - \frac{\partial W}{\partial x}\right) j + \left(\frac{\partial V}{\partial x} - \frac{\partial U}{\partial y}\right) k, \quad (40)$$

we can express in eqn. (40) as,

$$\nabla \times \mathbf{F} = \left(\nabla \cdot \mathbf{F}_{yz}^{*}\right) i + \left(\nabla \cdot \mathbf{F}_{zx}^{*}\right) j + \left(\nabla \cdot \mathbf{F}_{xy}^{*}\right) k, \tag{41}$$

where,

$$\mathbf{F}_{vz}^{*} = Wj - Vk, \tag{42}$$

$$\mathbf{F}_{zx}^* = Uk - Wi,\tag{43}$$

$$\mathbf{F}_{xy}^* = Vi - Uj. \tag{44}$$

Therefore,

$$\mathbf{C}_{xy}\mathbf{F} = \left(\mathbf{D}_{xy}\mathbf{F}_{yz}^{*}\right)i + \left(\mathbf{D}_{zx}\mathbf{F}_{zx}^{*}\right)j + \left(\mathbf{D}_{xy}\mathbf{F}_{xy}^{*}\right)k$$
(45)

$$C_{xyz} \mathbf{F} = \left(\mathbf{D}_{yz} \mathbf{F}_{yz}^{*}\right) i + \left(\mathbf{D}_{zx} \mathbf{F}_{zx}^{*}\right) j + \left(\mathbf{D}_{xy} \mathbf{F}_{xy}^{*}\right) k$$
(46)

are the two- and three-dimensional mimetic curls, respectively.

Compact Operators

High-order $(m \ge 4)$ mimetic operators can be represented in a "compact way" by factorizing the original matrices [25]. By doing this, we can attain higher orders of accuracy using only the smallest stencil,

$$\mathbf{D}_{kth} = \mathbf{D}_{2nd} \mathbf{R}_{kth},\tag{47}$$

where R_{kth} denotes the right factor matrix that when multiplied by the *2nd*-order divergence produces a *kth*-order **D** operator. The same can be done for the gradient,

$$\mathbf{G}_{kth} = L_{kth} \mathbf{G}_{2nd} \tag{48}$$

the reason why we factorize the divergence from the right and the gradient from the left is because in this way we can express the laplacian operator as follows:

$$\mathbf{L}_{kth} = \mathbf{D}_{2nd} R_{kth} L_{kth} \mathbf{G}_{2nd}$$
(49)

 \mathbf{L}_{kth} is our *kth*-order mimetic laplacian, and $R_{kth}L_{kth}$ is called the "star" operator (**S**). **S** can be seen as a tensor that contains properties that are inherent to each problem. The authors used compact representation of the CG operators to solve problems of acoustic wave propagation [6].

Accuracy Tests

Subject to.

We performed several accuracy tests to compare our fourth order operators with those defined [7]. In this section we show two of those tests in Figure 8,

$$F(x) = \log x + \cos x \tag{50}$$

The following tables show the magnitude of the error obtained with each method (Castillo-Grone and Corbino-Castillo) (Table 1).

Testing the laplacians with an elliptic problem (Table 2)

$$\nabla^2 f(x) = e^x,\tag{51}$$

$$\alpha f(0) - \beta f'(0) = 0, \qquad (52)$$

$$\alpha f(1) + \beta f'(1) = 2e \tag{53}$$

with α =1 and β =1. We obtained the following results.

As shown on Table 3 and Figure 9, the new mimetic laplacian

Page 4 of 6

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Figure 8: Comparison between continuous and discrete solutions. Visually, both discrete solutions are identical.

	Grad		
m	CG E ₂	CG E ₂	(∆ x) ⁴
10	0.0915	0.0204	0.6561
20	0.0066	0.0047	0.0410
40	0.0019	8.7e-4	0.0026
80	2.6e-4	1.0e-4	1.6e-4

Table 1: Comparing divergences.

	Gradient		
m			(∆ x) ⁴
10	0.0166	0.0174	0.6561
20	0.0018	0.0018	0.0410
40	4.4e-4	4.5e-4	0.0026
80	5.8e-5	5.9e-5	1.6e-4

Table 2:	Testing	the laplacians	with an	elliptic	problem
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operator is also considerably more precise than its CG counterpart (in some cases for up to two orders of magnitude).

	Gradient		
m		CG E ₂	(∆ x) ⁴
10	4.0e-5	1.2e-6	0.6561
20	4.3e-6	6.8e-8	0.0410
40	4.1e-7	9.5e-9	0.0026
80	3.8e-8	1.0e-9	1.6e-4

Table 3: The new mimetic laplacian operator.

These tests have been done using the Mimetic Operators Library Enhanced (MOLE) [24].

Conclusions

High order mimetic finite difference operators that satisfy a discrete extended Gauss-Divergence theorem have been presented. These operators have the same order of accuracy in the interior as well as the boundary, no free parameters and optimal bandwidth. They are constructed on staggered grids, using weighted inner products with a diagonal norm. Their construction using linear algebra illustrate the clarity of their formulation. A compact formulation, which uses the minimum second order stencils, has also been presented. These operators have been implemented in the open source mathematical library MOLE. Mimetic finite difference schemes using this operator produce excellent results on our test cases.

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Page 5 of 6

J Appl Computat Math, an open access journal ISSN: 2168-9679

Page 6 of 6

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