On second-order mimetic and conservative finite-difference discretization schemes

S. Rojas
Departamento de Física, Universidad Simón Bolívar, Venezuela
e-mail: srojas@usb.ve

J.M. Guevara-Jordan
Departamento de Matemáticas, Universidad Central de Venezuela, Venezuela
e-mail: juan.guevara@ciens.ucv.ve

Recibido el 24 de agosto de 2007; aceptado el 30 de enero de 2008

Although the scheme could be derived on the grounds of a relatively new numerical discretization methodology known as *Mimetic Finite-Difference Approach*, the derivation of a second-order mimetic finite difference discretization scheme will be presented in a more intuitive way, using Taylor expansions. Since students become familiar with Taylor expansions in earlier calculus and mathematical methods for physicist courses, one finds this approach of presenting this new discretization scheme to be more easily handled in courses on numerical computations of both undergraduate and graduated programs. The robustness of the resulting discretized equations will be illustrated by finding the numerical solution of an essentially hard-to-solve, one-dimensional, boundary-layer-like problem, based on the steady diffusion equation. Moreover, given that the presented mimetic discretization scheme attains second-order accuracy in the entire computational domain (including the boundaries), as a comparative exercise the discretized equations can be readily applied in solving examples commonly found in texbooks on applied numerical methods and solved numerically via other discretization schemes (including some of the standard finite-diffence discretization schemes).

Keywords: Mimetic discretizations; finite difference; partial differential equations; diffusion equation; Taylor expansions; boundary layer.

Aunque la derivación del esquema se puede realizar usando la reciente metodología de discretización numérica conocida como *Diferencias Finitas Miméticas*, estaremos presentando la derivación de un esquema de discretización mimético en diferencias finitas de segundo orden en una forma más intuitiva, mediante el uso de expansiones de Taylor. Considerando que los estudiantes se familiarizan con expansiones de Taylor en los primeros cursos de cálculo y métodos matemáticos para físicos, pensamos que la presente alternativa de presentar este nuevo esquema de discretización es más favorable de ser asimilada en cursos de computación numérica tanto de pregrado como de postgrado. La robusticidad del esquema será ilustrada encontrando la solución numérica de un problema unidimensional del tipo capa límite difícil de resolver en forma numérica y que se basa en la ecuación de difusión estacionaria. Más aun, dado que el esquema de discretización alcanza segundo orden de precisión en todo el dominio computacional (incluyendo las fronteras), como ejercicio comparativo el mismo puede ser rápidamente aplicado para resolver ejemplos comúnmente encontrados en textos sobre métodos numéricos aplicados y que se resuelven usando otras metodologías numéricas (incluyendo algunos esquemas de discretización en diferencias finitas).

Descriptores: Discretizaciones miméticas; diferencias finitas; ecuaciones diferenciales parciales; ecuación de difusión; expansiones de Taylor; capa límite (boundary layer).

PACS: 02.50.Ey; 82.20.Wt; 83.10.Pp; 83.10.Rs

1. Introduction

Numerical modeling of complex physical problems (*i.e.* turbulence, front tracking and so on) in sophisticated topological structures modeled by arbitrary grids, requires high-quality numerical schemes in order to be able to capture its fine details, which in turn implies high precision and accuracy in the numerical method in use [1, 2]. Accordingly, much effort has been devoted to creating a discrete analog of vector and tensor calculus that could be used to accurately approximate continuum models for a wide range of physical and engineering problems and that preserves, in a discrete sense, symmetries and conservation laws that are true in the continuum. Such an approach is therefore more likely to produce physically faithful results [3].

This endeavor has led recently to the formulation of a set of mimetic finite-difference discretization schemes to find high-order numerical solutions to partial differential equations that mimic underlying properties of the continuum differential operators including conservation laws, solution symmetries, fundamental identities of vector and tensor calculus [4, 5]. In particular, a recent article [6] shows a systematic way to construct high-order mimetic discretizations for the gradient and divergence operators, attaining the same order of approximation at the boundary and inner region. Discretizations with this feature have been considered challenging even in the simplest case of one dimension on a uniform grid. The framework of this mimetic approach is to build discrete versions of these operators satisfying a discrete analog of the divergence or Green-Gauss theorem

$$\int_{\Omega} \nabla\cdot(\vec{v}\, f)\, dV = \int_{\Omega} (\nabla\cdot\vec{v})\, f\, dV + \int_{\Omega} \vec{v}\cdot(\nabla f)\, dV = \int_{\partial\Omega} f\, \vec{v}\cdot d\vec{s}, \tag{1}$$

which implies that the discrete operators will satisfy a global conservation law. This condition also ensures that the discretization of the boundary conditions and that of the differential equation are compatible. In the case of one-dimensional discretizations, Eq. (1) takes the form of the familiar Fundamental Theorem of Calculus:

$$\int_0^1 \frac{dv}{dx} f\, dx + \int_0^1 v \frac{df}{dx} dx = v(1)f(1) - v(0)f(0), \qquad (2)$$

in which dv/dx plays the role of the divergence of the vector field $v(x)$, while df/dx plays the role of the gradient of the scalar field $f(x)$.

In this article we shall be presenting the derivation, via Taylor's expansions, of a second-order mimetic discretization scheme for the gradient and divergence operators [6]. Then, we can use the discretized scheme to build a second-order conservative scheme to numerically solve the diffusion equation. Though our presentation is much simpler and perhaps intuitive, it is not obvious by any means. In fact, the conservative scheme is obtained as a necessary first step in proving the convergence of the second-order mimetic scheme reported in [6]. Details of the proof can be found elsewhere [7, 8].

1.1. The continuum model problem

Being one of the most important and widely used equations in mathematical physics, the range of physical and engineering problems modeled by the diffusion equation (Eq. (3) below) includes heat transfer, flow through porous medium, and the pricing of some financial instruments. Accordingly, the wide range of applications of the diffusion equation somehow justifies the effort and time spent in finding ways to obtain high-quality numerical solutions to it in different contexts [9]. Correspondingly, the accuracy and robustness of our conservative discretization method will be shown by solving boundary-layer-like problems, which are modeled by the diffusion equation.

In terms of the invariant operators divergence ($\nabla\cdot$) and gradient (∇), the diffusion equation is written in the form

$$-\nabla \cdot (\overleftrightarrow{K}(\vec{x}) \cdot \nabla f(\vec{x})) = F(\vec{x}) \qquad (3)$$

where $\overleftrightarrow{K}(\vec{x})$ is a symmetric tensor, $f(\vec{x})$ is the target property we are looking for, and $F(\vec{x})$ is a source term. For instance, in a heat transfer problem, $\overleftrightarrow{K}(\vec{x})$, $f(\vec{x})$, and $F(\vec{x})$ are the thermal conductivity, the temperature, and a source of heat influencing the domain of interest, respectively; in a porous medium flow they are, respectively, the permeability tensor, the pressure driving the flow, and a source term (*i.e.* a producer or injector well in a oil field) affecting the fluid flow in the region of interest. In one dimension, Eq. (3) takes the form,

$$\frac{d}{dx}\left(K(x)\frac{df(x)}{dx}\right) = F(x), \qquad (4)$$

which, in terms of the discretized operators via the mimetic technique, is written in the form $\mathbf{D}(K\mathbf{G}f(x)) = F(x)$, where $\mathbf{D}$ and $\mathbf{G}$ are matrices representing the discretized version of the divergence and the gradient operators, respectively. That is, rather than discretizing a particular differential equation, the mimetic approach uses discrete operators to produce a discrete analog of the partial differential equations under consideration. In this form, once we have the discrete version of the differential operators of interest, one could discretize any equation written in terms of them. To have a boundary value problem properly expressed by Eq. (4), we shall impose boundary conditions of the Robin (mixed) type

$$\alpha_0 f(0) - f'(0) = \gamma_0; \quad \alpha_1 f(1) + f'(1) = \gamma_1 \qquad (5)$$

where α_0, α_1, γ_0 and γ_1 are known constants. It should be mentioned that finding reasonably accurate numerical solutions to partial differential equations by means of numerical schemes preserving key properties of the continuum (*i.e.* conservation laws; symmetry properties of the equation being discretized, and so on) has been an active research area [2]. Accordingly, many finite difference schemes can be found in the literature which are basically created for very specific problems [10]. On the other hand, in the present ongoing research on mimetic discretizations, the main effort is towards constructing high-order mimetic discretizations of differential operators, which are of general applicability rather than being limited to a specific problem.

2. Mimetic discretizations of D and G

In a general non-uniform *staggered* grid (Fig. 1) spanning the interval [0,1], the mimetic framework presented in [6] leads to the one-dimensional, second-order discretized mimetic $\mathbf{G}$ and $\mathbf{D}$, presented in Eqs. (6) [11]. From these equations and Fig. 1, it is clear that $\mathbf{D}$ is defined at cell points, but $\mathbf{G}$ at nodal points. It is important to bear in mind that these discretizations were obtained within the mimetic framework analysis reported in Ref. 6. Correspondingly, they satisfy the various conditions imposed by the mimetic approach mentioned in that article.

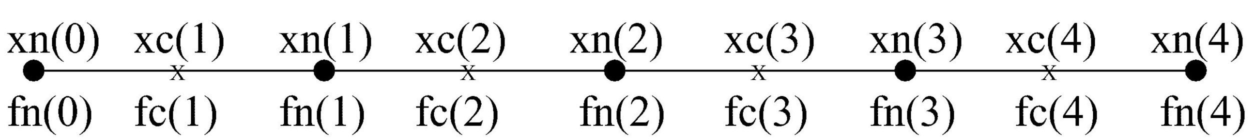

FIGURE 1. 1-D staggered (non-uniform point distributed) grid. The end points of each cell are the nodes $xn(i)$, the cells are indexed $xc(i) = (1/2)(xn(i) + xn(i-1))$. $f\alpha(j) \equiv f\alpha(x\alpha(j))$.

$$(\mathbf{G}f)_0 = -\left(\frac{xc(1)+xc(2)-2\,xn(0)}{(xc(1)-xn(0))\ (xc(2)-xn(0))}\right) fn(0) + \frac{-xc(2)+xn(0)}{(xc(1)-xc(2))\ (xc(1)-xn(0))} fc(1) + \frac{xc(1)-xn(0)}{(xc(1)-xc(2))\ (xc(2)-xn(0))} fc(2) \tag{6a}$$

$$(\mathbf{G}f)_1 = \frac{xc(1)+xc(2)-2\,xn(1)}{(xc(1)-xn(0))\ (-xc(2)+xn(0))} fn(0) - \left(\frac{xc(2)+xn(0)-2\,xn(1)}{(xc(1)-xc(2))\ (xc(1)-xn(0))}\right) fc(1) + \frac{xc(1)+xn(0)-2\,xn(1)}{(xc(1)-xc(2))\ (xc(2)-xn(0))} fc(2) \tag{6b}$$

$$(\mathbf{G}f)_i = -\frac{1}{xc(i+1)-xc(i)} fc(i) + \frac{1}{xc(i+1)-xc(i)} fc(i+1) \quad ; \quad i = 2, \cdots, N-2 \tag{6c}$$

$$(\mathbf{G}f)_{N-2} = -\frac{xc(N-1)-2xn(N-2)+xn(N-1)}{(xc(N-2)-xc(N-1))(xc(N-2)-xn(N-1))} fc(N-2) + \frac{xc(N-2)-2xn(N-2)+xn(N-1)}{(xc(N-2)-xc(N-1))(xc(N-1)-xn(N-1))} fc(N-1) - \frac{xc(N-2)+xc(N-1)-2xn(N-2)}{(xc(N-2)-xn(N-1))(xc(N-1)-xn(N-1))} fn(N-1) \tag{6d}$$

$$(\mathbf{G}f)_{N-1} = \frac{xn(N-1)-xc(N-1)}{(xc(N-2)-xc(N-1))(xc(N-2)-xn(N-1))} fc(N-2) + \frac{xc(N-2)-xn(N-1)}{(xc(N-2)-xc(N-1))(xc(N-1)-xn(N-1))} fc(N-1) - \frac{xc(N-2)+xc(N-1)-2xn(N-1)}{(xc(N-2)-xn(N-1))(xc(N-1)-xn(N-1))} fn(N-1) \tag{6e}$$

$$(\mathbf{D}u)_{i+\frac{1}{2}} = \frac{fn(i+1)-fn(i)}{xn(i)-xn(i-1)} \quad ; \quad i = 0, \cdots, N-1 \tag{6f}$$

2.1. Obtaining $\mathbf{D}$ and $\mathbf{G}$ via Taylor's expansions

Now, one would argue that the discretized scheme (6a)-(6f) could be obtained from a more intuitive point of view, using Taylor expansions and the benefit of hindsight. As is common when trying to obtain high-order finite-difference schemes and in perturbation theory, the starting anzat is not obvious, and the form in which we have intentionally presented Eqs. (6) will guide our insight.

In fact, the discretized gradient $(\mathbf{G}f)_0$ evaluated at the first $xn(0)$ node in the grid can be obtained by Taylor's expansion of the unknown $f(x)$ around $xn(0)$, and then evaluating the obtained expansion at the grid positions $xn(0)$, $xc(1)$ and $xc(2)$. Solving the resulting system of equations for the first derivative evaluated at $xn(0)$, equation (6a) is obtained.

By the same token, the discretized gradient $(\mathbf{G}f)_1$, equation (6b), is obtained by taking Taylor's expansion of $f(x)$ around $xn(1)$, and then evaluating the obtained expansion at the grid positions $xn(0)$, $xc(1)$ and $xc(2)$. The desired equation is found after solving the resulting system of equations for the first derivative evaluated at $xn(1)$.

Similar reasoning can be used to obtain Eqs. (6c)-(6e). The form in which the equations were written out will guide the reader in guessing the grid points around which Taylor's expansions should be carried out in order to obtain them. Equation (6f) is standard in finite differences.

Once we have a discretized set of equations for the divergence and gradient operators, one should check whether this scheme satisfies the desired properties implicit in the continuum version of the operators (conservation laws, symmetries and so on), which are required in order to be considered a mimetic discretization. As indicated, the set (6a)-(6f) already satisfies these conditions since they were first obtained in that context [6, 11].

TABLE I. Numerical Errors

Grid Size	Error Finite Difference	Error Support Operator	Error New Method
16	0.3958	0.1861	0.0794
64	0.2206	0.0154	0.0045
256	0.0717	0.0010	0.0002

2.2. From mimetic to conservative schemes

Reference [6] provides sufficient discussion about the desired properties that discretized forms $\mathbf{D}$ and $\mathbf{G}$ should satisfy in order to be considered a mimetic scheme. And following the systematic procedure outlined in that article, mimetic discretizations (6a)-(6f) were obtained, whose derivation via Taylor expansions were just presented.

Since one needs to solve the diffusion equation, the Laplacian operator is required. It turns out that a conservative scheme of our model problem (4) and (5) has the form

$$(\widehat{\mathbf{A}} + \mathbf{BG} + \widehat{\mathbf{D}}\mathbf{KG})f = b \tag{7}$$

In this expression $\mathbf{D}$ and $\mathbf{G}$ are matrix representations of the discretized scheme. $\widehat{\mathbf{D}}$ satisfies

$$\left(\widehat{\mathbf{D}}f\right)_0 = 0, \qquad \left(\widehat{\mathbf{D}}f\right)_n = 0,$$

and

$$\left(\widehat{\mathbf{D}}f\right)_{i+\frac{1}{2}} = (\mathbf{D}f)_{i+\frac{1}{2}}\,.$$

$\mathbf{B}$ is a boundary operator with only non-null entries $\mathbf{B}(1,1) = -1$ and $\mathbf{B}(n+2, n+1) = 1$. $\widehat{\mathbf{A}}$ is the $(n+2)\times(n+2)$ matrix having as non-zero entries those elements in its diagonal that correspond to boundary nodes ($\widehat{\mathbf{A}}(1,1) = \alpha_0$ and $\widehat{\mathbf{A}}(n+2, n+2) = \alpha_1$). $\mathbf{K}$ is a diagonal tensor whose known values are positive and evaluated at grid block edges.

$$f \equiv (f(x_0), f(x_{\frac{1}{2}}), f(x_{\frac{3}{2}}), \cdots, f(x_{n-\frac{1}{2}}), f(x_n))^T \tag{8}$$

$$b \equiv (\gamma_0, F_{\frac{1}{2}}, F_{\frac{3}{2}}, \cdots, F_{n-\frac{1}{2}}, \gamma_1)^T$$

This scheme is conservative and new. Its analysis has been recently developed in [7]. It is proved in [7], by an application of the modulus maximum principle, that the numerical scheme has an optimum second-order convergence rate.

2.3. An illustrative example

The one-dimensional boundary value problem in this test is formulated in terms of the ordinary differential equation

$$\frac{d^2 f}{dx^2} = \frac{\lambda^2 \exp(\lambda\, x)}{\exp(\lambda) - 1} \tag{9}$$

defined on the interval [0,1], and it's solution must satisfy Robin boundary conditions of the form

$$\alpha f(0) - \beta f'(0) = -1 \quad ; \quad \alpha f(1) + \beta f'(1) = 0 \tag{10}$$

at the borders. Equations (9) and (10) form together a well where problem for $\alpha = -\exp(\lambda)$, $\beta = (\exp(\lambda) - 1)/\lambda$, where λ an arbitrary non-null real number. This problem has a unique analytical solution given by $f(x) = (\exp(\lambda x) - 1)/(\exp(\lambda) - 1)$, and it represents a boundary layer for large values of λ. Correspondingly, it is an excellent test problem for evaluating numerical schemes with different discretization alternatives for boundary conditions.

In this test all the numerical methods were implemented on a uniform staggered grid. The value of the parameter λ was set equal to 20, although similar results and conclusions are obtained for any positive value of it. Numerical results are presented in Tables I, where we also show results obtained via two widely used discretizations schemes (finite-difference based on ghost point [10] and the mimetic support operator discretization described in Ref. 3)

Table I shows the numerical errors computed in the maximum norm. They indicate that on refined grids the new method achieved at least three exact digits in its approximation, while support operator and standard finite-difference methods obtained only two and one exact digits, respectively. Such results indicate a clear advantage to our new scheme.

3. Conclusion

Intended to be presented in applied numerical methods courses at both undergraduate and graduate levels, by means of intuitive Taylor expansions, an alternative complete derivation of a second-order mimetic discretization scheme for the divergence and gradient operators was presented. As illustrated via the diffusion equation, the scheme can be applied in building conservative discretization schemes of continuum problems formulated in terms of partial differential equations. The many advantages to conservative schemes in numerical studies have been known for some time and are still a fruitful research area. The results obtained from our test problem indicate a clear advantage to the presented new scheme over other widely used numerical discretization schemes. By using this approach, students can be introduced earlier to mimetic discretization and its advantages, particularly on the applications in the discretization presented here to physical, engineering and industrial problems.

1. S. Steinberg, *Comput. Meth. Appl. Math.* **4** (2004) 228.
2. F. Gibou and R. Fedkiw, *J. Comput. Phys.* **202** (2005) 577.
3. M. Shashkov, *Conservative Finite-Difference Methods on General Grids* (CRC Press, 2001).
4. J.E. Castillo, J.M. Hyman, M.J. Shashkov, and S. Steinberg, *Appl. Numer. Math.* **37** (2001) 171.
5. M. Lipnikov Shashkov and D. Svyatskiy, *J. Comput. Phys.* **211** (2006) 473.
6. J.E. Castillo and R.D. Grone, *SIAM J. Matrix Anal. Appl.* **252** (2003) 128.
7. J.M. Guevara-Jordan, S. Rojas, M. Freites-Villegas, and J.E. Castillo, *Divulgaciones Matemáticas* **13** (2005) 107.
8. J.M. Guevara-Jordan, S. Rojas, M. Freites-Villegas, and J.E. Castillo, *Advances in Difference Equations* (2007) 12303:1-12, www.hindawi.com/GetArticle.aspx?doi=10.1155/2007/12303
9. N. Robidoux, *Numerical Solution of the Steady Diffusion Equation with Discontinuous Coefficients*, Ph.D. Dissertation, University of New Mexico, Albuquerque, NM, 2002.
10. W.F. Ames, *Numerical Methods for Partial Differential Equations*, Third edition, 1993.
11. O. Montilla, C. Cadenas, and J.E. Castillo, To appear in *IMACS J. of Appl. Num. Math.*