Mimetic Opoerator Discretization 1D

Exploration of classical iterative methods and preconditioners

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Overview

Introduction

- Creating discrete approximations of partial differential equations is usually straightforward away from the boundary, but obtaining appropriate behavior on the boundary is rather complicated, even in the one-dimensional case.
- **Example:** Poisson equation

$$\nabla \cdot \nabla f = -F \tag{1}$$

$$\frac{d^2 f}{dx^2} = -F(x), \qquad x \in [0, 1] \qquad \text{(1-D)} \tag{2}$$

Mimetic operators

- Mimetic discretizations of differential operators are constructed to satisfy the discrete analogues of the continuous conservation identities, very important in Physics (conservation of mass, electric charge, etc.).
- Operators must be discretized using appropriate grids for scalar and vector fu

Mimetic operators (cont.)

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- **Example:** *Gauss' Divergence Theorem.* Given a region Ω of space, and its boundary $\partial\Omega$:

$$\int_{\Omega} \nabla \bullet (fv) dV = \int_{\partial\Omega} fv \bullet n dS \tag{3}$$

$$\int_{\Omega} (\nabla \bullet v) f dV + \int_{\Omega} v \bullet (\nabla f) dV = \int_{\partial\Omega} fv \bullet n dS \tag{4}$$

If $\Omega = [0,1] \in \mathbb{R}$ then the equation is reduced to integration-by-parts:

$$\int_0^1 \frac{dv}{dx} f dx + \int_0^1 v \frac{df}{dx} dx = v(1)f(1) - v(0)f(0) \tag{5}$$

Mimetic operators (cont.)

Constraints: The mimetic gradient ($G \equiv \nabla$), divergence ($D \equiv \nabla \bullet$), curl ($C \equiv \nabla \times$) and laplacian ($L \equiv \nabla^2 \equiv \Delta$) operators must follow:

- $Gf_{const} = 0$
- $Dv_{const} = 0$
- $CGf = 0$
- $DCv = 0$
- $DGf = 0$
- Conservation law by 4

Mimetic operators (cont.)

Condiciones: In 1-D, the operators must satisfy:

- $\frac{d}{dx} const. = 0$
- the Fundamental Theorem of Calculus: if a function f is continuous in an interval $[0, 1]$ then

$$\int_0^1 \frac{d}{dx} f(x) dx = f(1) - f(0) \tag{6}$$

- integration by parts:

$$\int_0^1 \frac{dv}{dx} f(x) dx + \int_0^1 v(x) \frac{df}{dx} dx = \; v(1)f(1) - v(0)f(0) \tag{7}$$

Staggered grid

Mimetic operators are defined on staggered grids. In this type of grids, scalar variables are stored in the centers of the cells; while vector components are placed on edges (or faces, in 3D).

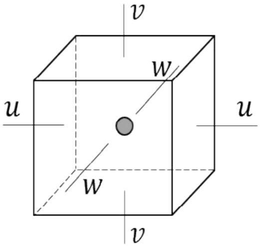

Figure: A 3D cell. *u*, *v* y *w* are the vector components used to calculate the divergence. In the case of rotational, we use the components that are tangential to the faces of the cell. **Ref.:** [Corbino and Castillo, 2020]

Discretization

- *Discrete divergence* acts on v, with v evaluated at the nodes and Dv evaluated at the centers.
- *The discrete gradient* acts on f, with f evaluated at the centers and Gf evaluated at the nodes.

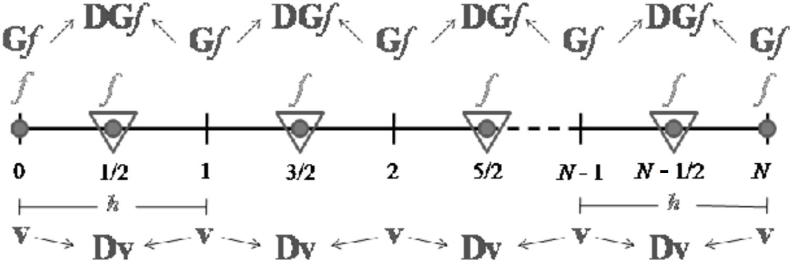

Figure: 1-D Staggered grid. **Ref.:** Castillo & Miranda, 2013.

Support operator method

For the discretization of the derivatives, centered finite differences might be used because they are of second order $O(h^2)$, except at the extremes -order $O(h)$- where we need forward finite differences (in x_0) and backwards (in x_N).

$$(Dv)_{i+\frac{1}{2}} = \frac{v_{i+1} - v_i}{h}, \qquad i = 0, 1, \cdots, N-1 \tag{8}$$

$$(Gf)_i = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h}, \qquad i = 0, 1, \cdots, N-1 \tag{9}$$

$$(Gf)_0 = \frac{f_{\frac{1}{2}} - f_0}{\frac{h}{2}}, \; (Gf)_0 = \frac{f_N - f_{N-\frac{1}{2}}}{\frac{h}{2}} \tag{10}$$

Support operator method (cont.)

If $v = (v_0, v_1, v_2, \cdots, v_N)^T \in \mathbb{R}^{N+1}$, then $Dv \in \mathbb{R}^N$ represents the approximation, at the centers of the cells, of $\nabla \bullet v$.

$$\begin{bmatrix} (Dv)_{\frac{1}{2}} \\ (Dv)_{\frac{3}{2}} \\ \vdots \\ \vdots \\ (Dv)_{N-\frac{1}{2}} \end{bmatrix} = \underbrace{\frac{1}{h} \begin{bmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & \cdots & \cdots & & \\ & & & \cdots & \cdots & \\ & & & & -1 & 1 \end{bmatrix}}_{\text{operador } D \in \mathbb{R}^{N\times(N+1)}} \begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ \vdots \\ v_N \end{bmatrix} \tag{11}$$

Support operator method (cont.)

If $f = (f_0, f_{\frac{1}{2}}, f_{\frac{3}{2}}, \cdots, f_{N-\frac{1}{2}}, f_N)^T \in \mathbb{R}^{N+2}$, then $Gf \in \mathbb{R}^{N+1}$ represents the approximation, at the nodes, of ∇f.

$$\begin{bmatrix} (Gf)_0 \\ (Gf)_1 \\ \vdots \\ (Gf)_{N-1} \\ (Gf)_N \end{bmatrix} = \underbrace{\frac{1}{h} \begin{bmatrix} -2 & 2 & & & & & \\ & -1 & 1 & & & & \\ & & \cdots & \cdots & & & \\ & & & \cdots & \cdots & & \\ & & & & -1 & 1 & \\ & & & & & -2 & 2 \end{bmatrix}}_{\text{operador G}\in\mathbb{R}^{(N+1)\times(N+2)}} \begin{bmatrix} f_0 \\ f_{\frac{1}{2}} \\ \vdots \\ \vdots \\ f_{N-\frac{1}{2}} \\ f_N \end{bmatrix} \tag{12}$$

Constraints on the operators

- Derivative of a constant function is zero. If $\mathbb{1}_d = (1, 1, \cdots, 1) \in \mathbb{R}^d$ y $c \in \mathbb{R}$ then:

$$D(c\mathbb{1}_{N+1}) = 0, G(c\mathbb{1}_{N+2}) = 0 \tag{13}$$

- Fundamental Theorem of Calculus (at the nodes):

$$< Dv, h\mathbb{1}_N >= v_N - v_0, \tag{14}$$

by midpoint integration rule.

- Fundamental Theorem of Calculus (in the centers):

$$< h\mathbb{1}_{N+1}, Gf >_P = h1_{N+1}^T PGf = f_N - f_0 \tag{15}$$

where $P = \text{diag}(1/2, 1, 1, \cdots, 1, 1, 1/2)$, by trapezoidal integration rule.

Constraints on the operators (cont.)

- Discrete integration by parts:

$$h < \hat{D}v, f > + h < Gf, v >_P = v_N f_N - v_0 f_0 \tag{16}$$

$$h < (\hat{D} + (PG)^T)v, f > = < Bv, f > \tag{17}$$

where $< x, y >= x_1 y_1 + \cdots + x_N y_N$ is the discrete analogue of the continuous inner product:

$$< f, g >= \int_0^1 f(x)g(x)dx \tag{18}$$

and

$$\hat{D} = \begin{bmatrix} 0 & & 0 \\ & D & \\ 0 & & 0 \end{bmatrix}, B = \begin{bmatrix} -1 & & & & \\ 0 & 0 & & & \\ & \ddots & \ddots & & \\ & & & 0 & 0 \\ & & & & 1 \end{bmatrix} \in \mathbb{R}^{(N+2)\times(N+1)} \tag{19}$$

The Castillo-Grone Method (CGM)

- Castillo and Grone [Castillo and Grone, 2003, Castillo and Miranda, 2013] proposed a method to builds differential operators of order k (for any k: even number), for **any** point of the grid (in the interior and in the border), without using ghost points.
- To achieve this goal, in addition to the matrix operators D and G, quadrature matrices Q and P and a boundary operator B are defined, which satisfy:

$$h < Dv, f >_Q + h < v, Gf >_P = < Bv, f > \tag{20}$$

- The CGM builds the gradient operator G in conjunction with the matrix P, and the divergence operator D in conjunction with the weight matrix Q. As a consequence of the equation 20, a new matrix B is generated.

The Castillo-Grone Method (cont.)

- A y A': matrices that approximate the derivatives on the boundary.
- M: band matrix that approximates the derivatives in the interior points.

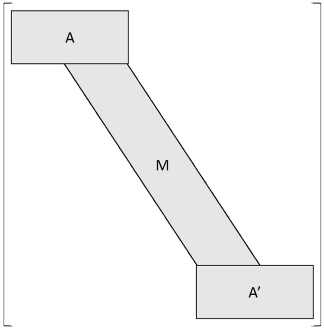

Figure: Taxonomy of a 1D differential operator, e.g. G gradient. **Ref.:** [Corbino and Castillo, 2020]

Operators of order $k = 2$

$$\begin{bmatrix} 0 & \frac{1}{4} & \frac{9}{4} \\ 0 & \frac{1}{4} & \frac{9}{4} \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \tag{21}$$

$$\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{22}$$

equivalen a

$$[x_1, x_2, x_3] = [-\frac{8}{3}, 3, -\frac{1}{3}], \tag{23}$$

$$[x_4, x_5] = [-1, 1] \tag{24}$$

$$\mathbf{G} = \frac{1}{h} \begin{bmatrix} \frac{-8}{3} & 3 & \frac{-1}{3} & & & \\ & -1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & -1 & 1 & \\ & & & \frac{1}{3} & -3 & \frac{8}{3} \end{bmatrix}$$

Figure: Taxonomy of a 1D gradient G operator. **Ref.:** [Corbino and Castillo, 2020]

Operators of order $k = 4$

We define A as a t-by-l matrix, $A' = P_t A P_l$, with $t = k$ and $l = (3/2)k$. Therefore, the general form of our desired $h\mathbf{D} = h\mathbf{D}(A)$ will look like

$$
h\begin{bmatrix}
 & & 0 & \cdots & & & & & & & \cdots & 0 \\
 & A & 0 & \cdots & & & & & & & \cdots & 0 \\
 & & 0 & \cdots & & & & & & & \cdots & 0 \\
0 & \cdots & 0 & s_1 & s_2 & \cdots & s_k & 0 & 0 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & \ddots & \ddots & \cdots & \ddots & 0 & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & 0 & s_1 & s_2 & \cdots & s_k & 0 & \cdots & 0 \\
0 & \cdots & & & & & & \cdots & 0 & & & \\
0 & \cdots & & & & & & \cdots & 0 & & A' & \\
0 & \cdots & & & & & & \cdots & 0 & & &
\end{bmatrix}. \tag{J.1}
$$

Figure: Taxonomy of a 1D -4th order- divergence operator. **Ref.:** [Castillo and Miranda, 2013]

Operators of order $k = 4$ (cont.)

Stencil central:

Consider a grid position x, and four surrounding grid points of the form $(x-(3/2)h)$, $(x-(1/2)h)$, $(x+(1/2)h)$, and $(x+(3/2)h)$. If we want to approximate $f'(x)$ in terms of $f(x-(3/2)h)$, $f(x-(1/2)h)$, $f(x+(1/2)h)$, and $f(x+(3/2)h)$ with local truncation error of $O(h^4)$, then it is necessary to find four coefficients $\sigma_1, ..., \sigma_4$, such that:

$$\sigma_1 f(x-\frac{3}{2}h)+\sigma_2 f(x-\frac{1}{2}h)+\sigma_3 f(x+\frac{1}{2}h)+\sigma_4 f(x+\frac{3}{2}h) = f'(x)+O(h^4). \quad \text{(J.14)}$$

Therefore, if we define the 1-by-4 matrix $\sigma = [\sigma_1\ \sigma_2\ \sigma_3\ \sigma_4]$, then

$$\sigma \begin{bmatrix} f(x-\frac{3}{2}h) \\ f(x-\frac{1}{2}h) \\ f(x+\frac{1}{2}h) \\ f(x+\frac{3}{2}h) \end{bmatrix} = f'(x) + O(h^4). \quad \text{(J.15)}$$

Figure: Solution of the 4th-order stencil at the center. **Ref.:** [Castillo and Miranda, 2013]

Operators of order $k = 4$ (cont.)

$$
\begin{bmatrix} f(x-\frac{3}{2}h) \\ f(x-\frac{1}{2}h) \\ f(x+\frac{1}{2}h) \\ f(x+\frac{3}{2}h) \end{bmatrix} = \begin{bmatrix} 1 & -\frac{3}{2} & \left(-\frac{3}{2}\right)^2 & \left(-\frac{3}{2}\right)^3 & \left(-\frac{3}{2}h\right)^4 \\ 1 & -\frac{1}{2} & \left(-\frac{1}{2}\right)^2 & \left(-\frac{1}{2}\right)^3 & \left(-\frac{1}{2}\right)^4 \\ 1 & \frac{1}{2} & \left(\frac{1}{2}\right)^2 & \left(\frac{1}{2}\right)^3 & \left(\frac{1}{2}\right)^4 \\ 1 & \frac{3}{2} & \left(\frac{3}{2}\right)^2 & \left(\frac{3}{2}\right)^3 & \left(\frac{3}{2}\right)^4 \end{bmatrix} \begin{bmatrix} f(x) \\ hf'(x) \\ h^2\frac{f''(x)}{2!} \\ h^3\frac{f'''(x)}{3!} \\ h^4\frac{f^{IV}(x)}{4!} \end{bmatrix} + \begin{bmatrix} O(h^5) \\ O(h^5) \\ O(h^5) \\ O(h^5) \end{bmatrix}
$$

$$
\triangleq V^T \begin{bmatrix} f(x) \\ hf'(x) \\ h^2\frac{f''(x)}{2!} \\ h^3\frac{f'''(x)}{3!} \\ h^4\frac{f^{IV}(x)}{4!} \end{bmatrix} + \begin{bmatrix} O(h^5) \\ O(h^5) \\ O(h^5) \\ O(h^5) \end{bmatrix}. \qquad \text{(J.17)}
$$

$$
\left(\frac{s}{h}\right) V^T = [0 \ (1/h) \ 0 \ 0 \ 0], \qquad \text{(J.21)}
$$

or

$$
Vs^T = [0 \ 1 \ 0 \ 0 \ 0]^T. \qquad \text{(J.22)}
$$

Figure: Solution of the 4th-order stencil at the center. **Ref.:** [Castillo and Miranda, 2013]

Operators of order $k = 4$ (cont.)

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This resulting equation is easily solved for

$$[s_1 \; s_2 \; s_3 \; s_4] = \left[\frac{1}{24} \; -\frac{9}{8} \; \frac{9}{8} \; -\frac{1}{24}\right], \tag{J.23}$$

which is exactly the 4th-order centered finite difference stencil.

Analogously, using Taylor's series and Vandermonde matrices will yield 4th-order accurate Castillo–Grone divergence near and at the boundary points.

Now that we have constructed the basic stencil

$$s = [s_1 \; s_2 \; s_3 \; s_4] = \left[\frac{1}{24} \; -\frac{9}{8} \; \frac{9}{8} \; -\frac{1}{24}\right], \tag{J.24}$$

Figure: Solution of the 4th-order stencil at the center. **Ref.:** [Castillo and Miranda, 2013]

Operators of order $k = 4$ (cont.)

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Stencil at the boundary:

Let $a_i = row_i(A)$, so that $a_1 = [a_{11}\ a_{12}\ a_{13}\ a_{14}\ a_{15}\ a_{16}]$, and so on.

$$V_1 a_1^T = V_2 a_2^T = V_3 a_3^T = V_4 a_4^T = [0\ 1\ 0\ 0\ 0]^T, \tag{J.3}$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -1/2 & 1/2 & 3/2 & 5/2 & 7/2 & 9/2 \\ (-1/2)^2 & (1/2)^2 & (3/2)^2 & (5/2)^2 & (7/2)^2 & (9/2)^2 \\ (-1/2)^3 & (1/2)^3 & (3/2)^3 & (5/2)^3 & (7/2)^3 & (9/2)^3 \\ (-1/2)^4 & (1/2)^4 & (3/2)^4 & (5/2)^4 & (7/2)^4 & (9/2)^4 \end{bmatrix} \begin{bmatrix} a_{11} \\ a_{12} \\ a_{13} \\ a_{14} \\ a_{15} \\ a_{16} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{J.8}$$

Figure: Solution of the 4th-order stencil at the boundary. **Ref.:** [Castillo and Miranda, 2013]

Operators of order $k = 4$ (cont.)

Stencil at the boundary

$$A(\alpha) = \Pi + \alpha\nu^T = \begin{bmatrix} -\frac{11}{12} & \frac{17}{24} & \frac{3}{8} & -\frac{5}{24} & \frac{1}{24} & 0 \\ \frac{1}{24} & -\frac{9}{8} & \frac{9}{8} & -\frac{1}{24} & 0 & 0 \\ 0 & \frac{1}{24} & -\frac{9}{8} & \frac{9}{8} & -\frac{1}{24} & 0 \\ 0 & 0 & \frac{1}{24} & -\frac{9}{8} & \frac{9}{8} & -\frac{1}{24} \end{bmatrix} +$$

$$\begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} [-1 \; 5 \; -10 \; 10 \; -5 \; 1]\,. \qquad \text{(J.13)}$$

Up to this point, $\mathbf{D}(A(\alpha))$ is a four parameter family of fourth-order accuracy everywhere, mapping from $\mathbb{R}^{(n+1)}$ to $\mathbb{R}^n$, as we will prove below.

Figure: Solution of the 4th-order stencil at the boundary. **Ref.:** [Castillo and Miranda, 2013]

Weight matrices P and Q

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4. Weight matrix P

The diagonal weight matrix P (from Eq. (6)) is obtained by:

$$\mathbf{G}^T p = b_{m+2}, \tag{17}$$

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 $\mathbf{G}$, the solution is $p = [\frac{3}{8} \ \ \frac{9}{8} \ \cdots \ 1 \ \cdots \ \frac{9}{8} \ \ \frac{3}{8}]^T$. System Eq. (17) is overdetermined but consistent. For our *4th*-order $\mathbf{G}$ (and $m = 20$), we get:

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

4.1. Weight matrix Q

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

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

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

$$q = \left[1 \ \frac{2186}{1943} \ \frac{1992}{2651} \ \frac{1993}{1715} \ \frac{649}{674} \ \frac{699}{700} \ \frac{18170}{18171} \ \frac{471744}{471745} \ 1 \ \cdots \right]^T. \tag{20}$$

Neither set of weights (p or q) must be recomputed for a different number of cells; however, the number of '1s' in the middle increases proportionally with m.

Figure: A method to obtain P and Q, for $k = 2$ y 4. **Ref.:** [Corbino and Castillo, 2020]

Future work

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- To build the 4th-order operators and analyze their structure.
- To reshape the matrices with modern (e.g. block) preconditioners.
- To test the (block?) linear systems with adaptive iterative methods, see `github.com/nidtec-una/krysbas-dev`.
- Current source code available at `github.com/gusespinola/mimetic-1dpoisson`.

Referencias

Castillo, J. E. and Grone, R. (2003).
A matrix analysis approach to higher-order approximations for divergence and gradients satisfying a global conservation law.
SIAM Journal on Matrix Analysis and Applications, 25(1):128–142.

Castillo, J. E. and Miranda, G. F. (2013).
Mimetic discretization methods.
CRC Press.

Corbino, J. and Castillo, J. E. (2020).
High-order mimetic finite-difference operators satisfying the extended Gauss divergence theorem.
Journal of Computational and Applied Mathematics, 364:112326.