High Order Mimetic Differential Operators

Jose E. Castillo, PhD

Computational Science Research Center San Diego State University San Diego, CA 92182-1245 www.csrc.sdsu.edu castillo@myth.sdsu.edu

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Abstract



- Mimetic Operators satisfy a discrete analog of the divergence theorem and they are used to create/design conservative/reliable numerical representations to continuous models.
- We will present a methodology to construct mimetic versions of the divergence and gradient operators which exhibit high order of accuracy at the grid interior as well as at the boundaries.
- Mimetic conditions on discrete operators are stated using matrix analysis and the overall high order of accuracy determines the bandwidth parameter.
- Test cases:
 - 2-D elliptic equations with full tensor coefficients
 - Elastic wave propagation under free surface and shear rupture boundary conditions

Outline



- Mimetic discretization
 - Principles/Foundations
 - Methodology of construction of mimetic operators
 - Second order and Higher order results
- Applications to elliptic problems and hyperbolic equations

Mimetic Discretization



- First order invariant continuum operators
 - div, grad, curl
- Discrete operators
 - DIV, GRAD, CURL
 - Preserve (exactly) many of the fundamental properties of the continuum differential operators (important to preserve conservation laws)

Goal



 Construct local high-order DIV, GRAD, CURL on uniform and non-uniform grids that mimic properties of continuum differential operators div, grad, curl

The Problem



- Find higher-order approximations GRAD, DIV to grad (∇) and div (∇·)
- Divergence Theorem

$$\int_{\Omega} \nabla \cdot \vec{v} f \, dV + \int_{\Omega} \vec{v} \nabla f \, dV = \int_{\partial \Omega} f \vec{v} \, \vec{n} \, dS$$

1-D Mimetic Operators

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Castillo & Grone (2003)

Discrete

DIV theorem

$$\langle \mathbf{D}v, f \rangle_Q + \langle v, \mathbf{G}f \rangle_P = \langle \mathbf{B}v, f \rangle$$
 (v, f are vectors)



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Higher-Order Case: Matrix Formulation



- Function v becomes an N-tuple
- Divergence operator, N by (N+1) matrix D
- If $e = (1, 1, \dots 1)^T$ then $\mathbf{D}e = 0$ can be expressed as $\mathbf{D}e = 0$
- Discrete analog of global conservation condition

$$\langle \mathbf{D}v, e \rangle = v_N - v_0$$

D has column sums equals –1, 0, ..., 0, 1,

$$e^{\mathrm{T}}\mathbf{D} = \begin{pmatrix} -1, & 0, & \cdots & 0, & 1 \end{pmatrix}^{\mathrm{T}}$$

Boundary Symmetry



Permutation matrix $P_k = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 & 0 \end{bmatrix}$

D should satisfy: $P_n \mathbf{D} P_{n+1} = -\mathbf{D}$ (Centro-skew-symmetric)

Summary of Matrix Conditions



- Consistency
- Mimetic/Column sums
- Local
- Interior symmetry
- Boundary symmetry

F	Fourth-Order Divergence													
	Find A	s.t.	H	=(A)	is a	a uni	form	ly 4 th	-orde	er DI\	/ ope	rato	or
			$\lceil A \rceil$					••••		0	0	0	0	
			0	0	0	$\frac{1}{24}$	$-\frac{9}{8}$	$\frac{9}{8}$	$-\frac{1}{24}$	0	0	0	0	
	H=H((A) =	0	0	0	0	$\frac{1}{24}$	$-\frac{9}{8}$	$\frac{9}{8}$	$-\frac{1}{24}$	0	0	0	
			0	0	0	0	0	$\frac{1}{24}$	$-\frac{9}{8}$	$\frac{9}{8}$	$-\frac{1}{24}$	0	0	
			0	0	0	0	0	0	$\frac{1}{24}$	$-\frac{9}{8}$	$\frac{9}{8}$	$-\frac{1}{24}$	0	
			0	0	0	0							A'	

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Conditions Near The Boundary



- a satisfies
 - Row sum

• Column sum
$$V_1 = V(1, -1, -3, -5, -7, -9)$$

Order constraints

• Where

$$V(1, -1, -3, -5, -7, -9) = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -3 & -5 & -7 & -9 \\ 1 & 1 & 9 & 25 & 49 & 81 \\ 1 & -1 & 27 & -125 & -343 & -729 \\ 1 & 1 & 81 & 625 & 2401 & 6561 \end{bmatrix}$$

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Conditions Near The Boundary (Cont'd)



Similarly

$$V_{2} = V(3, 1, -1, -3, -5, -7)$$

$$V_{3} = V(5, 3, 1, -1, -3, -5)$$

$$V_{4} = V(7, 5, 3, 1, -1, -3)$$

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Matrix Form of The Conditions



$$M = \begin{bmatrix} V_1 & 0 & 0 & 0 \\ 0 & V_2 & 0 & 0 \\ 0 & 0 & V_3 & 0 \\ 0 & 0 & 0 & V_4 \\ I_6 & I_6 & I_6 & I_6 \end{bmatrix}$$

$$b^{\mathrm{T}} = (0, -2, 0, 0, 0, 0, -2, 0, 0, 0, \cdots -1, 0, 0, -\frac{1}{24}, \frac{13}{12}, -\frac{1}{24})$$

 $M\mathbf{a} = b$

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Weighted Inner Product



• Find Q and D such that

$$\langle QDv, 1 \rangle = v_N - v_0$$

Or

$$e^{\mathrm{T}}QD = \begin{pmatrix} -1, & 0, & \cdots & 0, & 1 \end{pmatrix}^{\mathrm{T}}$$

New Formulation



$$\hat{V}(1, -1, -3, -5, -7, -9) = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 9 & 25 & 49 & 81 \\ 1 & -1 & 27 & -125 & -343 & -729 \\ 1 & 1 & 81 & 625 & 2401 & 6561 \end{bmatrix}$$

New Formulation (Cont'd)



$$\hat{M} = \begin{bmatrix} \hat{V}_1 & 0 & 0 & 0 \\ 0 & \hat{V}_2 & 0 & 0 \\ 0 & 0 & \hat{V}_3 & 0 \\ 0 & 0 & 0 & \hat{V}_4 \\ I_6 & I_6 & I_6 & I_6 \end{bmatrix}$$
$$\hat{M}\mathbf{a} = \hat{b}$$

• 3 parametric-
$$(\alpha, \beta, \gamma)$$
 family of solutions

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Fourth Order Operator D



	4751	909	6091	1165	129	25]
	5192	1298	15576	5192	2596	15576	
$D = \frac{1}{h}$	$\frac{1}{24}$	$-\frac{27}{24}$	$\frac{27}{24}$	$-\frac{1}{24}$	0	0	•••
	0	$\frac{1}{24}$	$-\frac{27}{24}$	$\frac{27}{24}$	$-\frac{1}{24}$	0	•••

Where the weights are

$$Q_0 = \frac{649}{576}, \quad Q_1 = \frac{143}{192}, \quad Q_2 = \frac{75}{64}, \quad Q_3 = \frac{551}{576}, \quad Q_4 = 1, \qquad Q_5 = 1, \qquad \cdots$$

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Fourth Order Operator G



	1152	10063	2483	3309	2099	697]
	407	3256	9768	3256	3256	4884	
$G = \frac{1}{h}$	0	$-\frac{11}{12}$	$\frac{17}{24}$	$\frac{3}{8}$	$-\frac{5}{24}$	$\frac{1}{24}$	
11	0	$\frac{1}{24}$	$-\frac{27}{24}$	$\frac{27}{24}$	$-\frac{1}{24}$	0	

• Where the weights are

$$P_0 = \frac{407}{1152}, \quad P_1 = \frac{473}{384}, \quad P_2 = \frac{343}{384}, \quad P_3 = \frac{1177}{1152}, \quad P_4 = 1, \quad \cdots$$

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First Results



Grids

- Staggered
- Nodal
- Weighted inner products
 - Diagonal matrix
- High order gradients
- High order divergence
- Higher dimensions/Tensor product grids

2-D Elliptic Problems (Huy Vu)



$$-div(K \operatorname{grad} u) = F(x), \quad x \in \Omega$$

- *K* is a tensor function, F(x) is a source term
- Robin boundary conditions

$$\beta(\hat{n}, K \operatorname{grad} u) + \alpha u = \gamma, \quad x \in \partial \Omega$$

• α , β , γ are function given on $\partial \Omega$

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Second Order Operators: D



Simplest case: Discrete divergence (D) defined by

$$(\mathbf{D}v)_{i+\frac{1}{2}} = \frac{v_{i+1} - v_i}{h}, \quad 1 \le i \le N - 1$$

$$\mathbf{D} = \frac{1}{h} \begin{bmatrix} -1 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & -1 & 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -1 & 1 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 1 \end{bmatrix} \in \mathbb{R}^{N \times (N+1)}$$

Second Order Operators: G



$$G = \frac{1}{h} \begin{bmatrix} -\frac{8}{3} & 3 & -\frac{1}{3} & 0 & \cdots & 0\\ 0 & -1 & 1 & \ddots & \ddots & \vdots\\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots\\ \vdots & 0 & -1 & 1 & 0\\ 0 & \cdots & 0 & \frac{1}{3} & -3 & \frac{8}{3} \end{bmatrix} \in \mathbb{R}^{(N+1) \times (N+2)}$$

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Second Order Operators: B



$$B = \begin{bmatrix} -1 & 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{8} & -\frac{1}{8} & 0 & 0 & \cdots & 0 \\ -\frac{1}{8} & \frac{1}{8} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \ddots & \cdots & 0 \\ & & \ddots & 0 & -\frac{1}{8} & \frac{1}{8} \\ & & 0 & \frac{1}{8} & -\frac{1}{8} \\ 0 & \cdots & 0 & 0 & 1 \end{bmatrix}$$

Second Order Operators: B (Cont'd)



$$B = QD + (PG)^{T}$$

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

$$Q = I$$

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Example 1: Dirichlet BCs



BVP:

$$-div(K grad u) = F(x, y) \quad \text{on} \quad (0,1) \times (0,1)$$

$$F(x, y) = -2(1 + x^{2} + xy + y^{2})e^{Xy}$$

$$K = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

Exact Solution:

$$u(x, y) = e^{xy}$$

Taken from: **"The Numerical Solution of Diffusion Problems in Strongly Heterogeneous Nonisotropic Materials**" by James Hyman, Mikhail Shashkov, and Stanly Steinberg.

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Results



	Mimetic	Method	Support Operator Method		
n	Mean Sqr Err	Max Err	Mean Sqr Err	Max Err	
3	1.89E-02	3.57E-02			
4	1.08E-02	2.25E-02			
5	7.00E-03	1.54E-02			
10	1.80E-03	4.40E-03			
17	6.21E-04	1.60E-03	1.06E-03	3.74E-03	
20	4.49E-04	1.20E-03			
33	1.66E-04	4.48E-04	2.58E-04	9.66E-04	
65	4.29E-05	1.18E-04	6.36E-05	2.45E-04	

Example 2: Dirichlet BCs



BVP:

$$-div(K grad u) = F(x, y) \text{ on } (0,1) \times (0,1)$$

$$F(x, y) = -\left[-22(y - y^2) - 26(x - x^2) + 18(1 - 2x)(1 - 2y)\right]$$

Tensor:

$$K = \begin{bmatrix} 11 & 9\\ 9 & 13 \end{bmatrix}$$

• Exact Solution: $u(x, y) = (x - x^2)(y - y^2)$ Taken from: **Mixed Finite Elements for Elliptic Problems with Tensor Coefficients as Cell-Centered Finite Differences.** Todd Arbogast, Mary F. Wheeler, and Ivan Yotov.

Results



	Mimetic	Method	Uniform cell-ce	entered Method
n	Mean Sqr Err	Max Err	Mean Sqr Err	Max Err
3	4.80E-03	7.80E-03	2.60E-01	
4	3.00E-03	5.40E-03	1.46E-01	
5	2.00E-03	3.90E-03	9.36E-02	
10	5.73E-04	1.20E-03	2.34E-02	
17	2.08E-04	4.43E-04	8.09E-03	
20	1.51E-04	3.25E-04	5.85E-03	
33	5.67E-05	1.23E-04	2.15E-03	
65	1.48E-05	3.31E-05	5.54E-04	

2-D Elastic Propagation With a Free Surface BC (Otilio Rojas)



Stress-Strain Relations define the symmetric stress tensor τ :

Parameters:

$$\rho \frac{\partial^2}{\partial t^2} \boldsymbol{u} = di\boldsymbol{v} \cdot (\boldsymbol{\tau} + \boldsymbol{m})$$

$$\boldsymbol{\tau} = \lambda (div\mathbf{u})\mathbf{I} + \mu (grad(\mathbf{u}) + grad(\mathbf{u})^{\mathrm{T}})$$

 $\lambda(x), \mu(x)$ $\rho(x)$ m(x,t)

 $\overline{}$

Lame's constants Density of the elastic medium Moment tensor of source distribution

Free-Surface BC:

$$\tau \cdot \vec{n} = 0$$

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Test Case: Lamb's Problem





Lamb's Problem Analitical solution in closed form (Cagniard-De Hoop's technique)



Results From Mimetic Schemes: H-MSSG, W-MSSG





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Dispersion Analysis: Rayleigh Wave





Spontaneous Rupture in Elastic Media



BCs: Spontaneous shear ruptures

 $\begin{cases} \tau - \tau_c \leq 0 & \text{(Shear traction doesn't exceed frictional strength)} \\ \vec{\tau} \, \dot{s} - \tau_c \, \dot{\vec{s}} = 0 & \Rightarrow \begin{cases} \dot{s} \left(\tau - \tau_c \right) = 0 & \text{(Slip rate non-zero if } \tau < \tau c \right) \\ \dot{\vec{s}} \tau = \dot{s}^{-} / \tau_c & \text{(Colinearity of traction and slip rate)} \end{cases}$

(Non-linear mixed BVP with an evolving boundary)

Constitutive Equations (Friction Laws)



$$\boldsymbol{\tau}_{c} = F(s, \dot{s}, \boldsymbol{\sigma}_{n}^{eff}, \boldsymbol{c}_{e}, \boldsymbol{\lambda}_{e}, \boldsymbol{T}, \boldsymbol{\Psi})$$

Slip-dependent:

Rate- and state-dependent:

$$F=F\bigl(s~\bigr)$$

Accounts for reduction of τc as slip increases (abrasion of asperities)

$$F = F\left(\dot{s}, \sigma_n^{eff}, \Psi \right)$$

Explain stick-slip behaviors seen in experiments

τ_{c}	maximum frictional strength on the fault		
	effective normal stress – includes effects of pore	S	slip
	fluids		slip rate
C_{e}	chemical effect of the fluid pressure	Т	temperature
λ_c	geometric characteristics of the fault surface (roughness)	Ψ	vector of state variables

Convergence: Fault Slip



Slip-dependent: Rate-and-state friction: Nc (Cohesive Zone Resolution) Nc (gridpoints per median cohesive width) 8.3 6.2 5 4.2 3.1 0.6 4 10^{2} 6 2 12.5 2.5 8.3 4.2 3.1 Δ 10⁰ 4th-mosn ~ 1.2 4th-mosn ~ 2.1 Δ ∇ MAX-RMS fault slip misfits (%) Final Slip Difference (%) ∇ Δ Δ 10 ð ∇ Δ DFM + ∇ ⊗ + Δ MOSN . 10⁻¹ ∇ ð ₽ 10⁰ ∇ ⊕ BIEM • X MOSN 4th-order 0 ዋ + MOSN mixed-order ∇ × 10⁻² \triangle MOSN 2nd-order (η =0.025) ÷ × MOSN 4th-order (cfl = $c^{*}(h)$) -2nd-order convergence 10⁻¹ х 20 0.05 0.1 0.2 0.3 0.4 0.5 30 40 50 60 80 100 Grid size (m) Grid interval (Km)

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4th Order MFD Yields

(Rojas et al, 2008-2009)



- Efficient modeling of Rayleigh-Pulse propagation along free surfaces
- Higher accuracy than second order solutions to rupture propagation problems
- Second-order convergence of rupture simulations on rate-and-state interfaces

Non-Uniform Operators G and D



Operators G and D

- Develop local transformations of the cells by using a "reference set of cells" in order to obtain local, mimetic operators G and D for non-uniform meshes.
- The Reference Set of Cells: RSC
 - The RSC is a set with two objects: one cell, called CD, for the construction of the divergence operator and two juxtaposed, uniform cells, called CG, for the construction of the gradient operator.

Weight Operators P and Q and Boundary Operator B (David Batista)



- Weight P and Q
 - The weight matrices for the generalized inner products are calculated based on a discrete version of the fundamental theorem of line integrals and a discrete Green identity that calculates the flux across the boundary.
- Boundary operator B
 - □ From the Stokes' theorem we get an expression for B, which is

 $B = \hat{D}^T Q + P G$

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2nd Order Non-Uniform Operators





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2nd Order Non-Uniform Operators (Cont'd Cont'd Cont

$$D = \begin{bmatrix} \frac{1}{J_{x_{j_{2}}}} & 0 & 0 & 0\\ 0 & \frac{1}{J_{x_{j_{2}}}} & 0 & 0\\ 0 & \frac{1}{J_{x_{j_{2}}}} & 0 & 0\\ 0 & 0 & \frac{1}{J_{x_{j_{2}}}} & 0\\ 0 & 0 & 0 & \frac{1}{J_{x_{j_{2}}}} \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & 0 & 0\\ 0 & -1 & 1 & 0 & 0\\ 0 & 0 & -1 & 1 & 0\\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

2nd Order Non-Uniform Operators



Weights for inner products

$$Q_{nu} = \hat{J}_D^{-1} Q_u, \qquad P_{nu} = P_u J_G^{-1}$$

• This technique produces the following result:

$$B_{nu} = \hat{D}_{nu}^{T} Q_{nu} + P_{nu} G_{nu} = B_{u}$$

Continuum Problem



$$-\nabla^{2} f(x) = F(x), \quad x \in [0,1]$$

$$\begin{cases} f(0) - f'(0) = b_{1} \\ f(1) + f'(1) = b_{2} \end{cases}$$

$$2 \times 10^{6} x$$

$$F(x) = \frac{2 \times 10^{7} x}{\arctan(100) (1 + 1 \times 10^{4} x^{2})^{2}}$$
$$b_{1} = \frac{100}{\arctan(100)} , \quad b_{2} = 1 + \frac{100}{\arctan(100) (1 + 1 \times 10^{4})}$$



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Numerical Results





Convergence Analysis



2 nd order operators						
Scheme	$E_h \ \cdot \ _{\infty}$	$E_h \ \cdot \ _{L_2}$				
Uniform	$112.6 \times h^{1.88}$	$129.4 \times h^{2.11}$				
Adapted	$1.3 \times h^{1.97}$	$1.1 \times h^{2.04}$				
Random	$19.82 \times h^{1.14}$	$19.0 \times h^{1.32}$				

4th order operators

Scheme	$E_h \ \cdot \ _{\infty}$	$E_h \ \cdot \ _{L_2}$
Uniform	$406438 \times h^{3.71}$	$665340 \times h^{3.99}$
Adapted	$119.4 \times h^{4.11}$	$44.3 \times h^{4.17}$
Random	$152.5 \times h^{1.52}$	$108.5 \times h^{1.52}$

Convergence Analysis (Cont'd)



$$E = c h^{p} + O(h^{p+1})$$
$$\left\| \hat{f} - f \right\|_{\infty} = \max \left\{ \hat{f}_{i+.5} - f_{i+.5} \right\|, \quad i = 1, ..., n \right\}$$
$$\left\| \hat{f} - f \right\|_{L_{2}} = \sqrt{\sum_{i=1}^{n-1} \left(\hat{f}_{i+.5} - f_{i+.5} \right) \left(J_{D}^{-1} \right)_{i,i}}$$

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2-D Boundary Layer Problem



$$-\nabla^{2} f(x, y) = F(x, y) \qquad (x, y) \in [0,1] \times [0,1]$$

$$F(x, y) = \frac{2 \times 10^{6}}{\arctan(100)} \left[\frac{x}{(1+1 \times 10^{4} x^{2})^{2}} + \frac{y}{(1+1 \times 10^{4} y^{2})^{2}} \right]$$

$$\alpha f(0, y) + \beta f'(0, y) = \frac{\arctan(100 y)}{\arctan(100)}$$

$$\alpha f(1, y) + \beta f'(1, y) = 1 + \frac{\arctan(100 y)}{\arctan(100)}$$

$$\alpha f(x, 0) + \beta f'(x, 0) = \frac{\arctan(100 x)}{\arctan(100)}$$

$$\alpha f(x, 1) + \beta f'(x, 1) = 1 + \frac{\arctan(100 x)}{\arctan(100)}$$

$$\alpha = 1 \qquad \beta = 0$$

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2-D Boundary Layer Problem (Cont'd)





High Order Mimetic Differential Operators





Current and Future Work



- 3-D/General grids
- Curl operator

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