High Order Mimetic Differences Methods

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Introduction

- Compatible Discretization Methods/Mimetic spectral element
  De Rahm Sequences, Differential Geometry, Exterior Calculus

- Mimetic Finite Difference Methods
  Summation By Parts - Scherer and Kreiss, 1974, generalized inner product, Nodal grids, Diagonal Norm 2-4-2

  Support Operators Methods -Samarskii/Shaskov, 1985, -Second Order, Staggered Grid

  Castillo-Grone 2003, Corbino-Castillo 2018 - 4-4-4
  Staggered Grids, Generalized inner products, Diagonal Norm

Motivation

- Most PDE's in Mathematical Physics are written using 1st order Operators gradient, divergence and curl.
- Mimetic discrete operators mimic the continuum ones by satisfying, in the discrete sense, the same properties that make them *more faithful* to the physics of the problem.

- Our Mimetic operators have *the same order* of approximation in the interior of the domain as at the boundary.

- Our mimetic operators have been used in many applications in a very successful way, making the schemes based on these operators *competitive* with the established ones.
- Staggered grids

- Time Discretizations
- Curvilinear Coordinates

Mimetic Discretization Methods

Mimetic operators are derived by constructing discrete analogs of the continuum operators from vector calculus, $\nabla\cdot, \nabla\times$ and ∇^2.

- Are discrete analogs of the continuum operator
- Satisfy vector calculus identities
- Satisfy global and local conservation laws
- Provide <u>uniform</u> order of accuracy

Mimetic Discretization Methods

These operators not only provide an uniform order of accuracy (all the way to the boundaries), but they also satisfy fundamental identities from vector calculus:

- Gradient of a constant $Gf_{const} = 0$
- Free stream preservation $Dv_{const} = 0$
- Curl of the gradient $CGf = 0$
- Divergence of the curl $DCv = 0$
- Divergence of the gradient $DG = L$

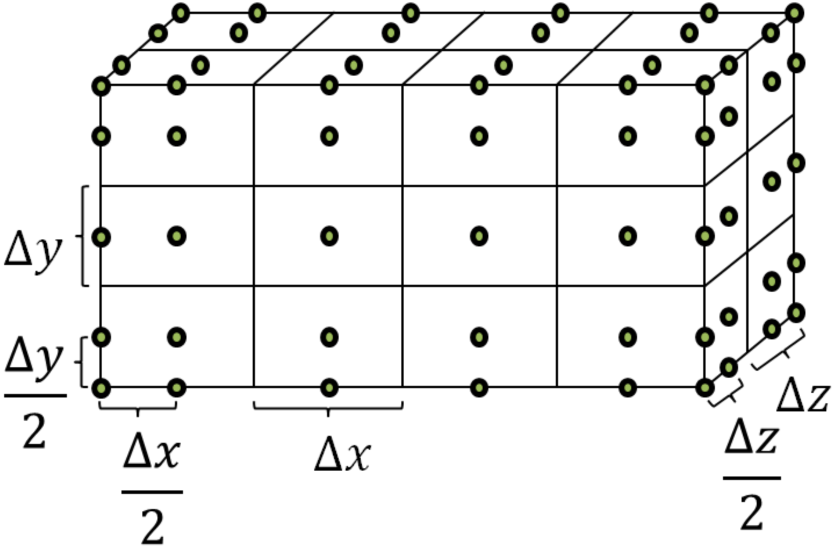
Extended Gauss Divergence Theorem

Mimetic operators

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

Mimetic weight matrices

3D Uniform Staggered Grid



MOLE (Mimetic Operators Library Enhanced)

MOLE is a software library that allows users to easily solve differential equations using mimetic discretization methods.

- Full support for sparse matrices operations
- It is available in C++ and MATLAB, and it only depends on Armadillo (An open source C++ linear algebra library)

All functions in MOLE return a sparse matrix representation of the corresponding mimetic operator.

Test Cases: 1D Wave

Test Cases: 2D Wave

Test Cases: Richards 1D

Test Cases: Membrane 2D

Compact Operators

Let D_2 and G_2 be the second order divergence and gradient.

Let R_k and L_k be matrices appropriate for (CGM) operators.

$M_k = D_2 R_k$ and $M_k = L_k G_2$ are mimetic difference operators of order k.

Then, explicit high-order accurate derivatives are

$$\left(\frac{\partial u}{\partial x}\right) = D_2\ R_k u \ \text{ or } \ \frac{\partial u}{\partial x} = L_k\ G_2 u,$$

Explicit R_4^G and R_4^D are given by

$$R_4^G = \begin{bmatrix} \frac{17958}{14245} & \frac{-8776}{14245} & \frac{154787}{341880} & \frac{-3415}{34188} & \frac{25}{9768} & & \\ \frac{-2}{35} & \frac{941}{840} & \frac{-29}{420} & \frac{1}{168} & & & \\ & \frac{-1}{24} & \frac{13}{12} & \frac{-1}{24} & & & \\ & & \frac{-1}{24} & \frac{13}{12} & \frac{-1}{24} & & \\ & & & \vdots & & & \\ & & & \frac{-1}{24} & \frac{13}{12} & \frac{-1}{24} & \\ & & & \frac{1}{168} & \frac{-29}{420} & \frac{941}{840} & \frac{-2}{35} \\ & & \frac{25}{9768} & \frac{-3415}{34188} & \frac{154787}{341880} & \frac{-8776}{14245} & \frac{17958}{14245} \end{bmatrix}$$

$$R_4^D = \begin{bmatrix} \frac{1045}{1142} & \frac{492}{2291} & \frac{-418}{2371} & \frac{328}{6821} & \frac{-25}{15576} & & & & & \\ \frac{-1}{24} & \frac{13}{12} & \frac{-1}{24} & & & & & & & \\ & \frac{-1}{24} & \frac{13}{12} & \frac{-1}{24} & & & & & & \\ & & & & \vdots & & & & & \\ & & & & & & \frac{-1}{24} & \frac{13}{12} & \frac{-1}{24} & \\ & & & & & \frac{-25}{15576} & \frac{328}{6821} & \frac{-418}{2371} & \frac{492}{2291} & \frac{1045}{1142} \end{bmatrix}.$$

Having

$$< Du, v >_Q + < u, Gv >_P = < Bu, v >$$

and letting $u = KGv$

we get

$$< DKGv, v >_Q + < KGv, Gv >_P = < BKGv, v >,$$

$$< DKGv, v >_Q + < Gv, Gv >_{PK} = < BKGv, v > .$$

Now if

$$-DKGf = F,$$

using fourth order operators $D_4,\ G_4$ we have

$$-D_4\ KG_4\ f = F.$$

If

$$D_4 = D_2\ R_4 \text{ and } G_4 = L_4\ G_2,$$

we get

$$-D_4\ KG_4\ =\ -D_2\ R_4\ KL_4\ G_2.$$

Here we have

$$-D_2\ S\ G_2\ f = F$$

with

$$S = R_4\ KL_4.$$

What is S?

$$S = \begin{pmatrix} A & & & & O \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ O & & & & A^* \end{pmatrix}$$

$$A^* = P_m \; A \; P_n$$

P_n are permutation matrices

for $K = I$,

S has non negative eigenvalues with only one zero eigenvalue and the rest positive eigenvalues.

Time Space

The standard continuous PDE is

$$T_0 \left\{ \left[\frac{\partial^2 u}{\partial x^2}(x, y, t) dx \right] dy + \left[\frac{\partial^2 u}{\partial y^2}(x, y, t) dy \right] dx \right\} =$$

$$\rho_0(x, y,) dxdy \frac{\partial^2 u}{\partial t^2}(x, y, t).$$

first order system for the unknowns $U_{i,j}(t),\ V_{i,j}(t)$

$$\begin{cases} \frac{dU_{i,j}}{dt}(t) & = & V_{i,j}(t) \\ \\ \frac{dV_{i,j}}{dt}(t) & = & \frac{1}{2} DGU_{i,j}(t) \end{cases}$$

$U_{i,j}(t)$ approximates $U(x_i, y_j, t)$ at (x_i, y_j), which is the center of (i, j)-th cell. The initial conditions are

$$\begin{cases} U_{ij}(0) & = & \sin(x)\ \sin(y) \\ V_{ij}(0) & = & 0 \end{cases}$$

To solve in time, discretize, calling $t_n = n\Delta t$, and $\Delta t = k$, and have position Verlet (2nd order) and Forest-Ruth (4th Order). Also, retain BC: $U_{ij}(t) = 0$, for cells sharing edge with $\partial\Omega$.

Table 1: Error for both the Position-Verlet and the Forest-Ruth algorithms.

$m = n$	$dx = dy$	Position-Verlet $\|E\|_2$	$\log_2(E_1/E_2)$	Forest-Ruth $\|E\|_2$	$\log_2($
51	0.2941	0.07724	–	0.0068	
101	0.1485	0.0221	2	0.0006	
201	0.0746	0.0049	2	$4.9e-5$	
401	0.0374	0.0014	2	$2.9e-6$	

3D-acoustic waves

Here, we transformed the linearized first order system which is not Hamiltonian into an equivalent first order systems which is Hamiltonian in nature. Then, we combine the space discretization using the uniformly accurate Mimetic difference operators with a high-order discrete time scheme based upon symplectic considerations.

We have the following manufactured solution at (x, y, z, t):

$$
\begin{aligned}
p &= \sin x \ \sin y \ \sin z \ \cos t \\
u &= -\cos x \ \sin y \ \sin z \ \sin t \\
v &= -\sin x \ \cos y \ \sin z \ \sin t \\
w &= -\sin x \ \sin y \ \cos z \ \sin t
\end{aligned}
$$

The first order system, not in Hamiltonian formulation, can be UNCOUPLED, yielding second order wave equations for each scalar unknown.

uncoupled for pressure

Initial Conditions for p are:
$p\ (x, y, z, 0) = \sin x\ \ \sin y\ \ \sin z$

$$\frac{\partial p}{\partial t} = \dot{p}\ (x, y, z, 0) = 0$$

Boundary Condition:
$p(x, y, z, t) = 0$ on all six faces of the cube $[0, \pi] \times [0, \pi] \times [0, \pi]$ for all $t \geq 0$.

Uncouple for velocity:

so that each scalar component of the velocity vector satisfies the scalar wave equation. In this case, we have a Robin Boundary Value Problem for each of these unknowns.

Consider for example the x-component of velocity, i.e. $u(x, y, z, t)$. Since $\frac{\partial u}{\partial x} = \sin x\ \sin y\ \sin z\ \cos t$,we see that on the pair of opposite faces $x = 0$ and $x = \pi$, the normal derivative of u vanishes there (so, a Neumann type on these faces).

But the function $u = -\cos x\ \sin y\ \sin z\ \sin t$ has a vanishing value on the other four faces of the cube:

$u = 0$ for $z = 0$ and $z = \pi$
$u = 0$ for $y = 0$ and $y = \pi$

3D Acoustic Wave - Pressure

3D Acoustic Wave - Velocity

Extended Gauss Divergence Theorem

Mimetic operators

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

Mimetic weight matrices

Mimetic Quadratures

1.0: INTRODUCTION

The numerical solution of partial differential equations (PDEs) obtained by preserving the properties of the original continuum differential operators is widely referred to as the Mimetic discretization methods. The spatial coordinates of the PDE can be discretized as divergence, gradient and curl that satisfy the underlying theorems of vector calculus (such as the Gauss Divergence theorem). These discretizations can then be used to solve higher order PDEs, Castillo et al [1]. Castillo [1] observed that the coefficient weights obtained for the 2nd order divergence Mimetic discretization method at the boundaries resemble those obtained from the Newton-Cotes formulation of numerical integration for ODE's. Navarro [2] compares the coefficients of higher order Newton-Cotes methods alongside with the equivalent Mimetic orders

Method Source	Newton Cotes	Navarro				Castillo et al	
Method Name	Newton	Mimetic	Mimetic	Newton	Newton	Mimetic	Mimetic
Reference Name	A	B	C	D	E	B1	C1
Coefficients	3/8, 9/8, ...	348/985, 473/384, 343/384, 612/599,...	1759/5586, 1224/877, 588/953, 2073/1657, 339/374, 746/735,...	1073/3527, 810/559, 343/640, 649/536,...	308/1123, 1499/880, -729/1783, 1899/596, -2716/2241, 1998/1021,...	407/1152, 473/384, 343/384, 1177/1152...	43531/138240, 192937/138240, 42647/69120, 86473/69120, 125303/138240, 140309/138240,...
# of function evaluations	4	8	12	8	12	8	12
Gradient order	2	4	6	4	6	4	6
Mimetic quadrature order	3	5	7	5	7	5	7

Table 1: shows the coefficients of the weights comparing the Newton-Cotes and Mimetic methods

The coefficients of the diagonal Weight matrix P associated to the high order mimetic gradient operator G, also satisfy the "exactness" sufficient conditions involving the Bernoulli numbers appearing in the Euler-Maclaurin Summation formula.

The classical divergence theorem states that the flux of a vector field v across the sectionally smooth boundary of a compact domain in two or three dimensions, equals the surface or volume integral of $div\ v$, and this integral, can then be regarded as a functional.

When dealing with quadrature approximations for integrals, we would then have a functional estimate for the domain integral, and it will be said to mimic the divergence theorem, when this estimate is accurate and also turns out to be equal to the quadrature over the domain's boundary.

2D Flux operator

2D Poisson Problem:

$$-\textbf{div}\ \mathbf{K}\ \textbf{grad}\ u = f, \qquad (x, y) \in V, \qquad K = \begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix}$$

2D Mimetic Gradient Operator:

$$G = \begin{bmatrix} G_x \\ G_y \end{bmatrix},$$

Mimetic Flux Operator:

$$\mathbf{G}^{\star} = -\mathbf{K}\ \textbf{grad} \cong -\mathbf{K}G = -\begin{bmatrix} \mathbf{K}G_x \\ \mathbf{K}G_y \end{bmatrix}$$

Where:

$$\mathbf{K}G_x = k_{xx}G_x + k_{xy}I_x(Gy),$$
$$\mathbf{K}G_y = k_{yy}G_y + k_{yx}I_y(Gx)$$

Problem 1: Full Tensor

- **Problem 1:**

$$-\textbf{div K grad } u = f, \qquad (x, y) \in V \quad \Omega = [0, 1]x[0, 1],$$

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

$$f(x, y) = -[22(y - y^2) - 26(x - x^2) + 18(1 - 2x)(1 - 2y)],$$

True solution (Dirichlet BC): $u(x, y) = (x - x^2)(y - y^2)$

Problem 1: Results

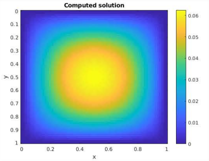


Figure 5: Computed solution for Problem 1: $-\mathbf{div}\ \mathbf{K}\ \mathbf{grad}\ u = f$

Table 1: Numerical results for problem 2, (using L_2 norm)

n	Mim. (2nd)	Mim. (4th)	Huy Vu	Supp. Operator
17	1.75E-04	4.38E-05	2.08E-04	8.09E-03
33	4.70E-05	6.31E-06	5.67E-05	2.15E-03
65	1.20E-05	8.49E-07	1.48E-05	5.54E-04

Problem 2: Full and Discontinuous Tensor

- **Problem 2:**

$$-\textbf{div}\ \mathbf{K}\ \textbf{grad}\ u = f, \qquad (x, y) \in \Omega$$

$$\Omega = [-1, 1]x[-1, 1]$$

$$\mathbf{K} = \begin{cases} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & x < 0 \\ \\ \alpha \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} & x > 0 \end{cases}$$

$$f(x, y) = \begin{cases} (-2 \sin y - \cos y)\alpha x + \sin y, & x < 0 \\ -2\alpha \exp(x) \cos y, & x > 0 \end{cases}$$

True solution: $u(x, y) = \begin{cases} (2 \sin y + \cos y)\alpha x + \sin y, & x < 0 \\ \exp(x) \cos y, & x > 0 \end{cases}$

Results for Problem 2, full and discontinuous tensor

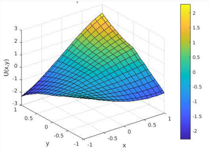


Figure 6: Computed solution for Problem 2: $-\textbf{div}\ \mathbf{K}\ \textbf{grad}\ u = f$

Numerical results for Problem 2: $-\textbf{div}\ \mathbf{K}\ \textbf{grad}\ u = f$

	New mimetic flux		Huy Vu		Supp. Oper.	
n	L_2 norm	Max norm	L_2 norm	Max norm	L_2 norm	Max norm
10	4.47E-04	1.10E-03	1.04E-02	1.02E-02		
14	2.07E-04	4.92E-04	5.30E-03	5.90E-03		
16	1.53E-04	3.51E-04	4.00E-03	4.70E-03	7.06E-03	
20	9.33E-05	1.97E-04	2.50E-03	3.40E-03		
32	3.46E-05	6.74E-05	9.75E-04	1.60E-03	1.73E-03	
64	8.75E-06	1.70E-05	2.39E-04	5.30E-04	3.96E-04	

Overlapping Grids

- A set of structured grids that overlap.
- Efficient for high-order methods.
- Efficiency of Cartesian grids with the accuracy of boundary fitted grids.
- High quality grids under large displacements.
- Smooth grids for accuracy at boundaries.

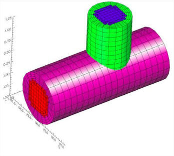


Figure 7: Overlapping Grid System for two intersecting pipes generated by Overture

Components of an Overlapping Grid System

- Backgroud cartesian grid G_1.
- Annular boundary fitted grid G_2
- Overlapping grid in physical space P.
- Grids in computational space C.

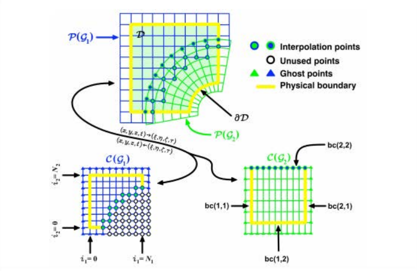


Figure 8: Simple Overlapping Grid System

Interpolation

Schemes: bilinear, biquadratic, trilinear, Lagrange, spline cubic.

Interpolation polynomial in the Lagrange form:

$$L(x) := \sum_{j=0}^{k} y_j \ell_j(x). \text{ Where: } \ell_j(x) := \prod_{\substack{0 \le m \le k \\ m \ne j}} \frac{x - x_m}{x_j - x_m}$$

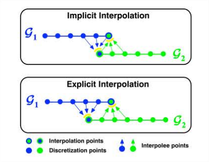


Figure 9: Implicit/Explicit Interpolation scheme for a one-dimensional overlapping grid system

Overlapping Grid System for Problem 2

$$\Omega = [0,1]x[0,1] = \Omega_1 \cup \Omega_2,$$

$$(x,y) \in \begin{cases} \Omega_1, & \text{if } (x-x_c)^2 + (y-y_c)^2 > r^2 \\ \Omega_2, & \text{otherwise} \end{cases}$$

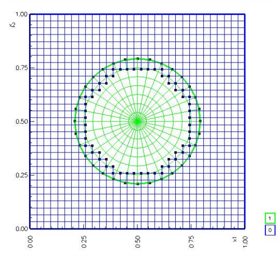
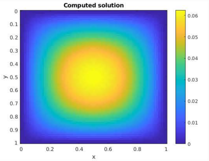


Figure 10: Overlapping grid system generated using Overture (Ogen) [3]

[3] $x_c = y_c = 0.5, r = 0.25$

Results for Problem 2, Full and Orthotropic Tensor



Numerical results for Problem 2: $-\textbf{div}\ \textbf{K}\ \textbf{grad}\ u = f$

n[4]	L_2-norm	Order(L_2)	Max-norm	Order(Max)
11	4.6893E-04		3.7857E-04	
16	1.0460E-04	3.1922	9.9572E-05	2.8415
32	1.3832E-05	2.9188	1.4216E-05	2.8082
64	1.7784E-06	2.9593	1.9257E-06	2.8841
80	9.1575E-07	2.9745	1.0056E-06	2.9116

[4] $n = n(\Omega_1) + n(\Omega_2)$

Richards Equation: Problem Formulation, Background

- Flow in the vadose zone has many complications as the parameters that control the flow are dependent on the saturation of the media, leading to a non-linear problem. This flow is referred as unsaturated flow and is described by Richards equation.
- Also known as the groundwater flow equation has a diffusion and an advection term.
- The advection term that is related to gravity and only acts in the z-direction.
- The Richards equation is a highly nonlinear problem.

Nonlinear functions: K, θ

Water content and hydraulic conductivity:

$$K(\psi) = K_s \frac{A}{A + |\psi|^\gamma}, \qquad \theta(\psi) = \frac{\alpha(\theta_s - \theta_r)}{\alpha + |\psi|^\beta} + \theta_r$$

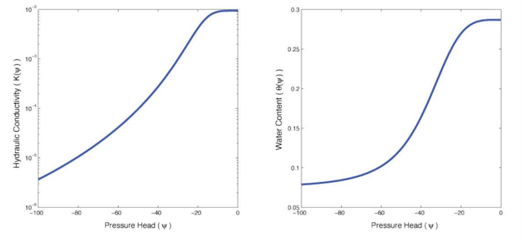


Figure 11: Van Genuchten curves for hydraulic conductivity and water content.

Parameters from [Celia et al., 1990]: $\alpha = 1.611x10^6, \theta_s = 0.287$, $\theta_r = 0.075, \beta = 3.96, A = 1.175x10^6, \gamma = 4.74, K_s = 9.44x10^{-3}$

Experiment

The initial conditions of a 40cm high 1D soil column are initially dry with a pressure head $\psi_0(x, 0) = 61.5$ cm. The boundary conditions applied are inhomogeneous Dirichlet with the top of the soil column $\psi(40cm, t) = 20.7cm$, and the bottom of the soil column $\psi(0cm, t) = 61.5cm$.
Numerical results by Cocket, R.[5]:

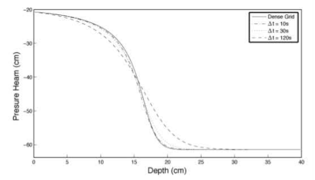


Figure 12: Solution of Richards Equation (FD, 1st order in general) at t = 360s

[5] Cockett, R. Simulation of Unsaturated Flow Using Richards Equation

Numerical Results

The obtained results showed excellent agreement between mimetic and finite difference approach presented by [Cocket, R.] at fixed Δt.

The discretization scheme (2^{nd} order in time, 4^{th} order space) was fully implicit and involved the use of Newtons iteration in order to deal with non-linearity.

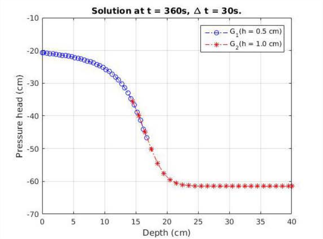


Figure 13: Richards Equation: MDM on Overlapping Grids

Extended Gauss-Divergence Theorem in Curvilinear Coordinates

$$\langle Du, v \rangle_Q + \langle u, Gv \rangle_P = \langle Bu, v \rangle \tag{1}$$

Let $\tilde{D}$ and $\tilde{G}$ denote the divergence and gradient in curvilinear coordinates. So, we have that,

$$\tilde{D} = J_D D \text{ and } \tilde{G} = J_G G, \tag{2}$$

Where J_D is the Jacobian corresponding to the divergence and J_G is the Jacobian corresponding to the gradient.
Hence,
$D = J_D^{-1}\ \tilde{D}$ and $G = J_G^{-1}\ \tilde{G}$
Using (2) in (1), we get
$\left\langle J_D^{-1} \tilde{D}\ u, v \right\rangle_Q + \left\langle u, J_G^{-1} \tilde{G} v \right\rangle_P = \langle Bu, v \rangle$

We have [**?**] that
$Q^T = J_D Q_{cc}$ and $P^T = J_G P_{cc}$, where Q_{cc} and P_{cc} are the corresponding weights for the operators in curvilinear coordinates.
So we get,

$$\left\langle J_D^{-1} \tilde{D}\ u, v \right\rangle_{[J_D Q_{cc}]^T} + \left\langle u, J_G^{-1} \tilde{G} v \right\rangle_{[J_G P_{cc}]^T} = \langle B\ u, v \rangle.$$

So, $\left\langle Q_{cc}\ J_D^T\ J_D^{-1} \tilde{D}\ u, v \right\rangle + \left\langle u,\ P_{cc}\ J_G^T\ J_G^{-1} \tilde{G} v \right\rangle = \langle B\ u, v \rangle.$

Which is, $\left\langle \tilde{D}\ u, v \right\rangle_{Q_{cc}} + \left\langle u, \tilde{G} v \right\rangle_{P_{cc}} = \langle B\ u, v \rangle.$

Since $B = B_{cc}$ as was demonstrated in [**?**],
we have $\left\langle \tilde{D}\ u, v \right\rangle_{Q_{cc}} + \left\langle u, \tilde{G}\ v \right\rangle_{P_{cc}} = \langle B_{cc}\ u, v \rangle.$

So, we have demonstrated that the mimetic operators $\tilde{D}, \tilde{G}$ in curvilinear coordinates satisfies the extended Gauss-Divergence Theorem and the corresponding "exactness condition" for the curvilinear discrete divergence.

Summary

Mimetic Finite Difference with Symplectic Integrators produce time and space accurate stable High Order Schemes for wave equations

Discrete energy conservation for 2D wave motion,2016

Discrete energy conservation for 3D acoustic waves 2018

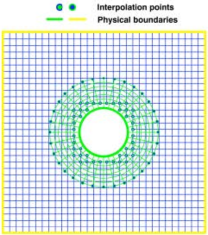
The coefficients of the diagonal weight matrix P for the mimetic high order mimetic gradient operator G, satisfy the "exactness" sufficient conditions involving the Bernoulli numbers appearing in the Euler-MacLaurin summation formula.

The Mimetic Quadratures satisfy the Divergence theorem. Mimetic

operators in curvilinear coordinates satisfy the Extended Gauss-Divergence Theorem

Current and future work

- Polygonal grids
- Unstructured grids
- Overlapping grids
- Time space mimetic differences
- Compact Operators



Mimetic Discretization Methods

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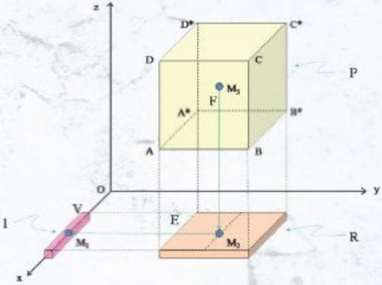
Guillermo F. Miranda



$$< \check{\mathbf{D}}\mathbf{u}, f >_Q + < \mathbf{u}, \check{\mathbf{G}} f >_P = < \mathbf{B}\mathbf{u}, f >$$

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