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Abstract

This document provides some crude comparison between mimetic differences and other numerical partial differential equation discretization methods. It is intended to show some examples where mimetic differences performs better than other methods in terms of computational time, accuracy and easiness of use. An more comprehensive and systematic illustration of the virtues of mimetic differences are going to be developed.

1 Introduction

Mimetic differences (MD) is a numerical method for constructing schemes for solving partial differential equations (PDEs). The following MD introduction follows from the general framework approach given in [18].

Mimetic differences (MD) were introduced by the work of [10]. The current variant of the mimetic operators that is implemented in the Mimetic Operators Library Enhanced (MOLE) [14] is the version made known by [13]. In both [10, 13] a one-dimensional (1D) non-periodic h-uniform staggered grid $X = X_C \cup X_N$ on $[a, b]$, composed of cell centers X_C (including $\{a, b\}$) and cell nodes X_N (including $\{a, b\}$, is utilized as the domain of scalar F and vector $\vec{V}$ discrete projections of the corresponding continuum fields $f, \vec{v}$. Discrete scalar fields F are defined on the dual mesh points (or cell centers X_C) while the discrete vector fields $\vec{V}$ are defined on the primal mesh points (or cell nodes X_N). Discrete analogs G, D of the gradient ∇ and divergence $\nabla\cdot$ vector calculus operators uniformly approximate the spatial partial derivatives with higher-order of accuracy $GF - \nabla f = \mathcal{O}(h^k), DV - \nabla \cdot \vec{v} = \mathcal{O}(h^k)$, $k = 2, 4, 6, 8$, in domains with boundary data. Utilizing these divergence D and gradient G discrete analogs high-order quadrature operators Q, P, for D, G respectively, are defined in such a way that the integration by parts formula (IBP) is approximated with the same order of accuracy of D, G, i.e., $\mathcal{B} = B + \mathcal{O}(h^k)$ since

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$B = D^T Q + PG$ and $V^T(B + \mathcal{O}(h^k))F = F(b)V(b) - F(a)V(a) = V^T \mathcal{B} F$, with

$$\mathcal{B} = \begin{pmatrix} -1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \cdots & \cdots & \vdots \\ & & \ddots & & \\ \vdots & \cdots & \cdots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix}.$$

It has been proven that Q, P obtained in this way are indeed high-order quadratures [1].

Kronecker products $\otimes$ allows the extension of D, G to two-dimensions (2D) and three-dimensions (3D) [11]. The introduction of high-order uniform mimetic interpolation operators $I^D : X_C \to X_N, I^G : X_N \to X_C$ [17] grants the approximation with high-order accuracy of the extended Gauss divergence theorem [16]. Discrete analog of Laplacian operators are defined as $L = DG$ and the discrete analog of the curl operator is defined utilizing the discrete analog of the divergence [11]. In practice, to incorporate boundary conditions to the Laplacian operator or in general to a second-order discrete analog of a linear operator one could add MOLE [24] functionalities. Furthermore, it has been shown that both high-order divergence and gradient discrete analogs can be written in compact form in terms of lower-order divergence and gradient discrete analogs, respectively [9].

Mimetic differences have also been extended for non-uniform grids in 1D [6], and 2D [8]. The same ideas can easily be extended to 3D. Mimetic differences can be extended to overlapping grids by utilizing overlapping grids from Overture [7] and from MOLE with Ogen and general interpolation operators [19].

It has been shown that MD operators obtained in this form satisfy the vector calculus identities [16] and that classic solutions of systems of conservation laws preserve mass, momenta, and energy [20]. Moreover, in the same work it is also demonstrated the preservation of those quantities for curvilinear coordinates.

2 Comparison with finite differences

In this section it is mentioned current comparisons with finite differences in terms of accuracy, execution time and easiness to use.

2.1 1D Wave equation

In [23] example 10.1 states the following problem: Use the finite-difference method to solve the wave equation for a vibrating string

$$u_{tt} = 4\, u_{xx} \qquad \text{for } 0 < x < 1 \text{ and } 0 < t < 0.5,$$

with the boundary conditions

$$\begin{aligned} u(0,t) = 0 \qquad \text{and} \qquad u(1,t) = 0 \qquad & \text{for } 0 \le t \le 0.5, \\ u(x,0) = f(x) = \sin(\pi x) + \sin(2\pi x) \qquad & \text{for } 0 \le x \le 1, \\ u_t(x,0) = g(x) = 0 \qquad & \text{for } 0 \le x \le 1, \end{aligned}$$

whose exact solution is $u(x,t) = \sin(\pi x)\,\cos(2\pi t) + \sin(2\pi x)\,\cos(4\pi t)$.

In [4], Armoa solves the same problem utilizing mimetic differences 1D Laplacian operator of second-order together with a Leapfrog scheme. There are a couple of videos displaying the fact that the mimetic approximation visually matches the exact solution while the finite difference solution utilizing MATLAB can be clearly distinguished from the exact solution. It also provides an accuracy comparison between the tho methods which is summarized in the following tables.

Method	Mean Square Error	Maximum Error	L_2-norm
Finite Differences	0.002393	0.177220	0.035363
Mimetic Differences	0.000001	0.002941	0.000733

Table 1: Accuracy comparison for 50 cells.

Method	Mean Square Error	Maximum Error	L_2-norm
Finite Differences	0.000006	0.009241	0.001757
Mimetic Differences	0.000000	0.000008	0.000002

Table 2: Accuracy comparison for 1000 cells.

One can clearly see in Tables 1, and 2, that no matter the number of uniform cells utilized, finite differences posses at least a couple of orders of magnitude smaller mean square error, maximum error and L_2-norm error.

The source MATLAB code can be found in Github [5].

2.2 Fractional derivatives

In [21], Mardo et al., solve the fractional problem

$$c\,\varrho\,\frac{\partial^\alpha u}{\partial t^\alpha}(x,t) = \lambda\,\frac{\partial^2 u}{\partial t^2}(x,t) + g(x,t), \qquad (x,t) \in [0,L]\times[0,T],$$

where $\frac{\partial^\alpha u}{\partial t^\alpha}$ is the Caputo fractional derivative of order $\alpha \in (0,1)$ defined as

$$\frac{\partial^\alpha u}{\partial t^\alpha}(x,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial u}{\partial s}(x,s)\,(t-s)^{-\alpha}\,ds, \qquad 0 \le t \le T.$$

The initial conditions are

$$u(x,0) = f(x), \qquad x \in [0,L],$$

and the Neumann-Robin type boundary condition for $t \in [0,T]$

$$\left\{\begin{array}{rcl} -\lambda\,\frac{\partial u}{\partial x}(0,t) &=& q(t), \\ -\lambda\,\frac{\partial u}{\partial x}(L,t) &=& h(t)(u(L,t) - u^\infty), \end{array}\right.$$

where c is the specific heat, λ is the thermal conductivity coefficient, ϱ is the density, h is the heat transfer coefficient, u^∞ is the environment temperature and q is the heat flux.

	$\|E(\Delta x, \Delta t)\|_\infty$			
Grid ($\Delta x \times \Delta t$)	t = 0.75		t = 1.00	
	IFD	MD	IFD	MD
$\frac{1}{100} \times \frac{1}{100}$	0.00414288	0.00190269	0.01080850	0.00423427
$\frac{1}{100} \times \frac{1}{200}$	0.00146142	9.34982209E-04	0.00384188	0.00224898
$\frac{1}{100} \times \frac{1}{300}$	7.73882266E-04	5.76161563E-04	0.00205081	0.00141923

Table 3: Variation of the approximation maximum norm error for the Implicit Finite Difference and the Mimetic Difference scheme with different time refinement level Δt.

The following table shows the maximum norm error for both the Implicit Finite Difference (IFD) and the Mimetic Differences (MD) at time $t = 0.75$ and $t = 1.00$.

It can be seen from Table 3, that the error decreases when the time step Δt is reduced. This behavior is expected as MD is second-order in time while IFD is first-order only, which supports the proposal numerical schemes for fractional order PDEs.

	$\|E(\Delta x, \Delta t)\|_\infty$			
Grid ($\Delta x \times \Delta t$)	t = 0.75		t = 1.00	
	IFD	MD	IFD	MD
$\frac{1}{100} \times \frac{1}{100}$	0.00414288757	0.0019026870	0.010808523	0.0042342705
$\frac{1}{200} \times \frac{1}{100}$	0.004195998	0.0019008641	0.0109263755	0.0042278331
$\frac{1}{300} \times \frac{1}{100}$	7.73882266E-04	5.76161563E-04	0.00205081	0.00141923

Table 4: Variation of the approximation maximum norm error for the Implicit Finite Difference and the Mimetic Difference scheme with different space grid refinement level Δx.

It can be seen from Table 4, that the error slowly decreases when the grid size Δx is reduced for MD. However, the same does not happen for IFD. Here the error increases due to round off errors, when one reduces the grid size Δx. This behavior is expected as MD is second-order in time while IFD is first-order only, which supports the proposal numerical schemes for fractional order PDEs.

2.3 FitzHugh-Nagumo equations

In this example it is show a case when MD is several times faster than Finite Differences.

In [26] Rubio and Verão, solve the FitzHugh-Nagumo system in Ω for $t > 0$ given by

$$\begin{aligned} \frac{du}{dt} &= D\,\Delta u - u(u-\alpha)(u-1) - w + I_{ext}, \\ \frac{dw}{dt} &= \epsilon(u - \gamma w), \end{aligned}$$

where u represents the excitability of the system (related to a $[K^+]$-voltage), w is a recovery variable which represents combined forces that tend to return to cell membrane rest, I_{ext} is the magnitude of an external stimuli applied to a neuron which triggers excitation, D is the diffusion coefficient, and $0 < \epsilon \ll 1$ describes time scale proportion between variables u and w.

Neurons	FD	MD
128	0.2075	0.0474
256	1.9502	0.2221
512	27.5378	4.2444
1024	470.6450	100.4102

Table 5: CPU time in seconds for both finite differences (FD) and mimetic differences (MD).

By looking at Table 5, one can notice that on both cases an explicit time discretization was utilized. One can estimate that MD requires only a fifth of the time needed by FD finish the simulation.

2.4 Reaction-Diffusion equations

In [2], the authors have to solve a system of three nonlinear equations describing the stem cell, nutrient and chemokine dynamics on a three dimensional. The equations of the model are given by

$$\begin{aligned} s_t &= \nabla \cdot (D_s \nabla s - \chi (\nabla q) s) + \mu_{\max} \frac{(1+k)n}{k n_{\max} + n} \left(1 - \frac{s}{s_{\max}}\right) s - R_d s, \\ n_t &= \nabla \cdot (D_n \nabla n) - \delta_{\max} \frac{n^4}{\theta^4 + n^4} s \\ q_t &= \nabla \cdot (D_q \nabla q) - R_{sq} s q - R_q q. \end{aligned}$$

Each of the equation has initial and boundary conditions. The authors were not able to use some software packages such as COMSOL but they found simple to use MOLE. The next is the first paragraph of section 3.1 of their paper :

"In this paper, given that our model includes a new variable, a new partial differential equation and its respective boundary conditions, we opted for high-order mimetic methods, based on finite differences, which are easy to implement. Our proposal was to show that, with mimetic differences, it is possible to find a numerical solution to our coupled system of partial differential equations."

3 Comparison with finite elements

In this section it is mentioned current comparisons with the family of finite elements methods in terms of accuracy, and execution time.

3.1 Elastodynamics

In [15], De La Puente et al., compare Discontinuous Galerkin (DG) and Mimetic Differences is several aspects for the velocity-stress formulation of the elastodynamics equations for the 3D

isotropic case with a curvilinear domain utilizing a fully staggered grid approach. The equations read as follows

$$\begin{aligned}
\frac{\partial}{\partial t}\sigma_{xx} - (\lambda+2\mu)\frac{\partial u}{\partial x} - \lambda\frac{\partial v}{\partial y} - \lambda\frac{\partial w}{\partial z} &= 0,\\
\frac{\partial}{\partial t}\sigma_{yy} - \lambda\frac{\partial u}{\partial x} - (\lambda+2\mu)\frac{\partial v}{\partial y} - \lambda\frac{\partial w}{\partial z} &= 0,\\
\frac{\partial}{\partial t}\sigma_{zz} - \lambda\frac{\partial u}{\partial x} - \lambda\frac{\partial v}{\partial y} - (\lambda+2\mu)\frac{\partial w}{\partial z} &= 0,\\
\frac{\partial}{\partial t}\sigma_{xy} - \mu\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) &= 0,\\
\frac{\partial}{\partial t}\sigma_{yz} - \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) &= 0,\\
\frac{\partial}{\partial t}\sigma_{xz} - \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) &= 0,\\
\rho\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\sigma_{xx} - \frac{\partial}{\partial y}\sigma_{xy} - \frac{\partial}{\partial z}\sigma_{xz} &= 0,\\
\rho\frac{\partial v}{\partial t} - \frac{\partial}{\partial x}\sigma_{xy} - \frac{\partial}{\partial y}\sigma_{yy} - \frac{\partial}{\partial z}\sigma_{yz} &= 0,\\
\rho\frac{\partial w}{\partial t} - \frac{\partial}{\partial x}\sigma_{xz} - \frac{\partial}{\partial y}\sigma_{yz} - \frac{\partial}{\partial z}\sigma_{zz} &= 0,
\end{aligned}$$

where λ is the first Lamé constant and μ is the shear modulus. Parameter ρ is the density, the normal stress components are given by $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$, and the shear stresses are $\sigma_{xy}, \sigma_{yz}, \sigma_{xz}$. The components of the particle velocities are denoted by u, v, w.

These equations are constrained by a free-surface condition with topography. Both DG and MD have similar statistics in the different tests. On one hand DG can be applied to unstructured grids than MD. On the other hand MD is much faster than DG in deformed grids. This can be seen in the Table 4 of the paper which can be summarized in the next table.

Method	Phase misfit	Envelope misfit	Relative CPU cost
DG	0.00%	0.00%	×12
MD	1.93%	4.82%	×1

Table 6: Comparison of relative computing cost and average errors obtained for all the receivers. The model size and propagation time were identical for all solutions. This comparison assumes DG solution as the reference to compare to.

One can clearly see in Table 6, that the MD solution averaged on all receivers is close to the DG solution. However, it is on average 12 times faster than DG.

3.2 Anisotropic Diffusion

In [3], Arbogast et al., solved the following steady state anisotropic diffusion equation (qualified as relatively hard by the authors)

$$-\nabla\cdot\Gamma\nabla u = f,$$

where Γ is a symmetric positive definite matrix that represents a diffusion or conductivity tensor, f is a forcing function. In particular, examples 6.2 of their paper is with

$$\Gamma = \begin{pmatrix} 11 & 9 \\ 9 & 13 \end{pmatrix},$$

with exact solution given by $u = (x - x^2)(y - y^2)$ and Dirichlet boundary conditions.

In [9], Boada et al., solve the same problem utilizing MD. The next table compares the accuracy of both solutions measured in terms of the exponent of h the mesh size.

Method	h exponent
Mixed FEM	1.50
MD (2^{nd}-order)	1.90
MD (4^{th}-order)	2.80

Table 7: Converge error rate as an exponent of the mesh size h for the anisotropic Laplacian equation with Dirichlet boundary conditons. The number of cells is close to 20.

One can observe in Table 7, that the error mesh size exponent is better for MD than for Mixed FEM.

3.3 Allen-Cahn equations

In [25], Orizaga et al., solved the non-linear parabolic Allen-Cahn PDE. It reads as

$$u_t = \Delta u - \frac{1}{\epsilon^2} f(u).$$

One inhomogeneous two-component material concentration is used to represent the Allen-Cahn system using the order parameter u, which is a scalar function for one phase. Values $u = \pm 1$ are corresponding to the two distinct phases. Within the interfacial area, the order parameter u exhibits a constant yet sharp variation from one phase to the next across the phase interface. The thickness of the interfacial region is directly related to small $\epsilon > 0$.

The authors of the paper compare MD with the *pdepe* MATLAB built-in function for solving several 1D and 2D Allen-Cahn equations with periodic and non-periodic boundary conditions. The following are some paragraphs of the Conclusion section of their paper.

"In this paper, we investigated and implemented a numerical method that is based on a mimetic finite difference operator for solving different variants of the nonlinear Allen-Cahn equation with periodic and non-periodic boundary conditions. In addition, we also analyzed the performance of the mimetic-based numerical method by applying it to the classical heat equation with a variety of boundary conditions. We evaluated the performance of the mimetic-based numerical method by comparing the errors of its solutions with those obtained by a classical finite difference method and the *pdepe* built-in Matlab function. We computed the L^1 errors of the numerical solutions by using the exact solutions when they are available or with the reference solutions obtained for a refined mesh. We adapted the mimetic-based numerical method by using the MOLE library. Some few adaptations were needed in order to deal with the Allen-Cahn equation in

one dimension due to the specific boundary conditions of the examples. We presented several results with regard to errors and numerical convergence tests in order to provide insight into the reliability and accuracy of the mimetic-based numerical method. The numerical results show that the method based on the mimetic difference operator is a reliable method for solving the Allen-Cahn and heat equations with both periodic and non-periodic boundary conditions. Moreover, the mimetic-based method shows an order of convergence as good as the finite difference method and better than the *pdepe* Matlab function. On the other hand, the numerical results show that the *pdepe* Matlab function solutions seem to preserve a fixed level accuracy for small time step values, but the associated errors don't decrease for smaller time step sizes. We also found that the solutions generated by the mimetic-based method are more accurate than the ones generated by the *pdepe* Matlab solver provided that the time step is small enough ($h \approx 10^{-3}$). Similar errors between the mimetic and finite difference approach were found when considering the second order approximation. However, when considering high order approximation the mimetic approach was superior in accuracy and ease of implementation (while requiring small amount of number of cells N) since reaching higher order is accomplished very efficiently due to the optimized MOLE libraries.

We also combined the mimetic finite difference operator with an energy stable splitting method to solve the Allen-Cahn equation in 2D. In particular, we utilize the convexity splitting approach coupled with the mimetic finite difference method using random initial states. This initial condition enables us to model the problem of phase separation process of two materials. The results showed that this approach is numerically reliable and is capable to describe the correct dynamics for the Allen-Cahn equation by ensuring the energy decreasing property. Finally, the results presented in this study show that the mimetic finite-difference operator or the MOLE library is a reliable tool to solve the Allen-Cahn equation and it is promising for other phase field models. The MOLE library is an open source and can be modified to adapt to the particular phase field model and can be easily implemented with higher order accuracy."

4 Comparison with support operator method

In this section it is mentioned current comparisons with finite differences in terms of accuracy.

4.1 Laplacian

In [12], the authors compare the accuracy of solving the following Poisson equation with MD and the Support Operator Method (SOM).

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

with Robin boundary conditions

$$\begin{aligned} \alpha\, f(0) - \beta\, f^{'}(0) &= -1, \\ \alpha\, f(1) + \beta\, f^{'}(1) &= 0, \end{aligned}$$

where

$$F(x) = \frac{-\lambda\, e^{\lambda x}}{e^{\lambda} - 1}, \qquad \alpha = -e^{\lambda}, \qquad \beta = \frac{e^{\lambda} - 1}{\lambda}, \qquad \lambda = -1.$$

The following table describes the comparison between MD and SOM in terms of accuracy for this problem.

h	SOM	MD (with B)	MD (with $\mathcal{B}$)
0.20	0.0053750	0.0013814	0.0010364
0.10	0.0014693	0.0003246	0.0002596
0.05	0.0003870	0.0000774	0.0000675

Table 8: Average component-wise absolute deviations from the problem solution.

Table 8 implies that the two versions of the mimetic differences (with the boundary operator B and with the exact boundary operator $\mathcal{B}$) achieve more accurate solutions than that of the support operator method.

4.2 Anisotropic Diffusion

In [22] Hyman et al., solve the following problem

$$-\nabla \cdot K\nabla u = f, \qquad (x, y) \in V.$$

Here V is a 2D region, K is a symmetric positive definite matrix, f is a forcing function. The boundary conditions are general Robin (or mixed),

$$K\nabla u \cdot \vec{n} + \alpha\, u = \psi, \qquad (x, y) \in \partial V,$$

where $\vec{n}$ is the unit outer normal to the boundary ∂V, and α, ψ are functions on ∂V.

In Problem 1 of the paper, the authors solve the case when the permeability K is given by

$$K = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},$$

with exact solution given by $u = e^{xy}$ and forcing term $f(x, y) = -2(1 + x^2 + xy + y^2)\, e^{xy}$.

The same problem is solved by Boada et al. [9] utilizing MD. The following table compares the accuracy of both SOM and MD.

h	MD (with 2^{nd}-order G)	MD (with 4^{th}-order G)	SOM
1/16	8.46E-04	1.86E-04	3.74E-03
1/32	2.29E-04	2.80E-05	9.66E-04
1/64	6.00E-05	6.11E-06	2.45E-04

Table 9: Maximum errors.

Looking at Table 9, it is evident that MD is more accurate than SOM for this problem.

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