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Mimetic Difference Schemes Preserve Mass, Momenta and Energy for Systems of Conservation Laws in Curvilinear Structured Grids

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Abstract

The following document demonstrates mimetic difference schemes preserve mass, momenta, and energy for systems of conservation laws given in structured meshes including curvilinear domains. The proofs utilize a general framework where properties of the different mimetic operators are derived from a high-order discrete analog of the extended Gauss divergence theorem, without specifying actual matrix representations of the divergence and gradient operators.

1 Introduction

Mimetic methods for numerically solving partial differential equations (PDEs) aim to construct schemes that utilize discrete analogs of first-order vector calculus differential operators that, besides convergence and accuracy, aim to replicate properties of the continuum model such as symmetries and conservation of some quantities. What features and relationships to mimic are what differ among mimetic methods. Mimetic techniques are of two types: those which derive all its properties from vector calculus integral theorems or those that focus reproducing some calculi identities and from there obtain all operator characteristics and relationships. In the first set one finds [22, 4, 7, 6]. In the second, examples of methods that elaborate a discrete vector calculus [20], tensor calculus [7, 17], exterior calculus [1, 18, 3], and others based on algebraic topology [14, 15], as well as geometric and structure-preserving methods [21], can be found in the literature.

The first mimetic method to achieve high-order accuracy was published in [4]. In particular, MD methods attain uniform accuracy they achieve over the whole computational domain, including near boundary grid points, a property that no other numerical method for solving PDEs has been able to exhibit.

This paper is about mimetic difference (MD) [4, 6] approaches which target to reproduce in the discrete realm a high-order approximation of the one-dimensional (1D) integration by parts (IBP) formula and from there the extended Gauss Divergence Theorem [10]. These two methods begin by introducing a staggered grid and defining on it specific high-order divergence and gradient matrix representations D and G, respectively. Then, utilizing those discrete analogs, attempt to satisfy a high-order approximation of the IBP formula. This objective triggers the introduction of high-order inner product weights Q and P associated to the divergence and the gradient, respectively [19]. Moving forward from one-dimension (1D) to higher dimensions via Kronecker products reveal the need to introduce interpolation operators I^D and I^G to be able to reproduce basic algebraic operations among the different discrete analogs applied to projections of scalar and vector fields [8]. Later on, it has been demonstrated that the matrix representation of the mimetic operators hold

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discrete analogs of vector calculus identities [10] and that the divergence and gradient generalized inner product Q and P are indeed quadrature weights [23]. Moreover, it has been exhibited that mimetic schemes can be shown to converge for some PDEs [11] and mass and energy convergence for some PDEs [9, 11, 12].

A general framework for formulating mimetic difference methods, that do not require specifying explicitly discrete analogs of the divergence and gradient differential operators can be found in [13]. This procedure utilizes only the sizes of the matrix representations D and G of the divergence and gradient, respectively, and aims to satisfy with high-order of accuracy the IBP formula. Accomplishing this task demands the introduction of inner product weights Q, P and establishes some relationships between D, G, Q, P. Splitting computational grid points into three different set points, introduces some direct decomposition in D and G, which through the relationships with Q and P, translates into direct decomposition and properties in the structure of Q and P. Moreover, it can also shown that these decompositions are reflected onto splitting of I^D and I^G. Furthermore, it has been shown that MD derived utilizing the general framework satisfy vector calculus identities and that positive diagonal weights Q and P are indeed quadrature weights.

This paper proves that mimetic difference schemes preserve quantities in the discrete sense that are expected to be conserved for general systems of conservation laws on curvilinear structured grids. Among these quantities one finds for example mass, energy, momentum. The proofs utilize the general framework of [13]. The document proceeds in the following way. Section 2 summarizes some properties of the mimetic operators that the general frame is able to derive. Sections 3 demonstrate the preservation of quantities for general system of conservation laws. Section 5 provides some conclusions.

2 The general frame for high-order mimetic differences

The following is a summary of the general frame for presenting the derivation of MD approaches. It focuses on the discrete analog of the IBP formula, and obtains the main properties of the one-dimensional (1D) operator discrete analogs without explicitly finding them. These properties replicate in the discrete realm the Fundamental Theorem of Calculus (FTC).

2.1 One-dimensional mimetic differences

The general frame for MD approaches is introduced for 1D first.

2.1.1 The staggered grid

In $[-1, 1]$, MD utilizes a mesh of N uniform cells and a staggered grid. The staggered grid is composed of a face grid that contains the edges of the cells (or nodes)

$$X_F = \left\{ x_l = -1 + \frac{2l}{N},\ 0 \leq l \leq N \right\},$$

and a center grid, that includes all center cells and domain boundary points,

$$X_C = \{-1\} \cup \left\{ x_{l+\frac{1}{2}} = -1 + \frac{1}{N} + \frac{2l}{N},\ 0 \leq l \leq N-1 \right\} \cup \{1\}.$$

Notice that the cardinalities of both X_F and X_C are different. The gradient G, and divergence D, discrete analogs should be mappings such $G : X_C \to X_F$, $D : X_F \to X_C$. Therefore the non-square matrix representations of G and D are of orders $(N+1)\times(N+2)$ and $(N+2)\times(N+1)$, respectively.

In addition, since the gradient of a scalar constant field should be the zero vector field, discretization of this property imposes that if $G = [G_{ij}]$, $1 \leq i \leq N+1$, $1 \leq j \leq N+2$, then $G\mathbb{1} = \vec{0}$, where $\mathbb{1} = (1, \cdots, 1) \in \mathbb{R}^{N+2}$. Similarly, the divergence of a constant vector field is zero and hence $D\,\vec{\mathbb{1}} = 0$, where $\mathbb{1} = (1, \cdots, 1) \in \mathbb{R}^{N+1}$. Moreover, since the divergence is not computed at the boundaries, the first and last rows of D are zero. The Laplacian discrete analog is defined by $L = D\,G \in \mathbb{R}^{(N+2)\times(N+2)}$.

Moreover, MD operators are chiefly constructed to approximate with high accuracy the integration by parts formula (IBP) for 1D scalar field f and 1D vector field $\vec{v}$,

$$\int_U \vec{v} \cdot \nabla f \; dU + \int_U f \, \nabla \cdot \vec{v} \; dU = \int_{\partial U} f \, \vec{v} \cdot \vec{n} \; dS. \tag{1}$$

The high-order discrete IBP formula requires that

$$\langle DV, F \rangle + \langle V, GF \rangle = V_N F_N - V_0 F_0,$$

where $V = v_{|X_F}, F = f_{|X_C}$, are the projections of v, f to the finite grids, respectively, and the angular brackets mean that the integrals are approximated utilizing a classic quadrature. However, this is not possible to achieve [19] unless special weighted inner products are introduced, meaning the need of MD diagonal weights $P \in \mathbb{R}^{(N+1)\times(N+1)}$ and $Q \in \mathbb{R}^{(N+2)\times(N+2)}$, such the following identity is attained with high-order accuracy,

$$\langle DV, F \rangle_Q + \langle V, GF \rangle_P = V_N F_N - V_0 F_0. \tag{2}$$

If in (2), one assumes the constant scalar field $F = \mathbb{1} \in \mathbb{R}^{(N+2)\times 1}$, then $G\mathbb{1} = \vec{0}$ implies

$$h\,\mathbb{1}^T QD = (-1, 0, \cdots, 0, 1). \tag{3}$$

If in (2), one assumes the constant vector field $V = \mathbb{1} \in \mathbb{R}^{(N+1)\times 1}$, then $D\vec{\mathbb{1}} = 0$ implies

$$h\,\mathbb{1}^T PG = (-1, 0, \cdots, 0, 1). \tag{4}$$

2.1.2 Additional structure to D and G

It is shown in [13] that one can decompose as direct sums the 1D operators D and G, if one uses appropriates stencils for X_F and X_C, respectively. This direct sum triggers the following splitting of the 1D inner product weights Q and P, respectively,

$$Q = \left[\begin{array}{c|c|c} Q_0^k & & \\ \hline & I_{N+2-2\bar{b}} & \\ \hline & & Q_N^k = (Q_0^k)^F \end{array}\right], \qquad P = \left[\begin{array}{c|c|c} P_0^k & & \\ \hline & I_{N+1-2\bar{b}} & \\ \hline & & P_N^k = (P_0^k)^F \end{array}\right],$$

for I_m identity matrix of order m, provided one utilizes symmetric stencils with respect to the 1D boundaries and where the F superscript refers to the operation of flipping rows followed by flipping columns of a matrix.

2.2 Weights Q and P as high-order quadratures

One naturally wonders if non-negative weights $\{w_l\}$ can be used for general quadratures in the sense of approximating $\int_{x_0}^{x_N} g(x)\,dx$, for a smooth function g, i.e.,

$$(1,\cdots,1)h\,W g \approx \int_{x_0}^{x_N} g(x)\,dx,$$

where g is the projection of the function $g(x)$ onto a grid $[x_0,x_1,\cdots,x_N]$ and with $W=P$, or $W=Q$, with $W=\mathrm{diag}(W_L,I,W_R)$, $W_L=\mathrm{diag}(w_1,\cdots,w_{\bar{b}}), W_R=\mathrm{diag}(w_{\bar{b}},\cdots,w_1)$ and I an appropriate square identity matrix.

Without loss of generality, one can assume enough differentiability for g, and hence there exist a smooth function $G(x)$ such $g(x)=G^{'}(x)$. In that case,

$$(1,\cdots,1)h\,W g \approx \int_{x_0}^{x_N} g(x)\,dx = \int_{x_0}^{x_N} G^{'}(x)\,dx = G(x_N)-G(x_0). \tag{5}$$

Notice that formula (5) is verified by Q for vector fields V (see (3)) and satisfied by P for scalar fields F (see (4)).

2.3 Some mimetic difference operator properties in d-dimensions

In $[-1,1]^d$, MD utilizes m_l cells along axis X_l, $l=1,\cdots,d$. The staggered grid is composed of cell centers and cell vertices X_C, and of cell centered faces X_F, given respectively by

$$\begin{aligned} X_F &= \bigcup_{j=1}^{d}\left[\left(\prod_{l<j}(X_C^j\setminus\{-1,1\})\right)\times X_F^j\times\left(\prod_{l>j}(X_C^j\setminus\{-1,1\})\right)\right],\\ X_C &= \prod_{j=1}^{d} X_C^j. \end{aligned}$$

Extensions of the 1D divergence D, gradient G, and inner product weight operators Q and P are built by utilizing Kronecker products of the 1D operators and some near identity matrices of convenient orders (see [13, 10]).

3 Mass and energy preservation for systems of conservation laws

Given the following sets

$$I=\{1,\cdots,c\},\qquad J=\{1,\cdots,d\},\qquad L=[-1,1]^d,\qquad L_0=[-1,1]^{d-1},\qquad K=[0,T],$$

consider the system of c conservation laws in d-dimensions, with $x=(x_1,\cdots,x_d)$, and the unknown $u(x,t)=(u_1(x,t),\cdots,u_c(x,t))^T$, and initial condition $u^0(x)=(u_1^0(x),\cdots,u_c^0(x))^T$, that are described by

$$\begin{aligned} u_t+\mathrm{div}(F(u)) &= 0_{c\times 1}, & (x,t)&\in \mathring{L}\times\mathring{K}, \\ u(x,0) &= u^0(x), & x&\in L, \end{aligned} \tag{6}$$

with $\mathring{L} = int(L)$, the interior of L, and that hold boundary conditions given by

$$\begin{aligned} u_i(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d,t) &= g_i^-(x_1,\cdots,x_{j-1},x_{j+1},\cdots,x_d,t), \quad i\in I, j\in J,\\ u_i(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d,t) &= g_i^+(x_1,\cdots,x_{i-1},x_{i+1},\cdots,x_d,t), \quad i\in I, j\in J, \end{aligned}$$

where $g_i^{\pm} : L_0 \times K \to \mathbb{R}^c$, $i = 1,\cdots,c$, are smooth functions. The flux F is given by

$$F(u) = \begin{pmatrix} F_{11}(u) & \cdots & F_{1d}(u) \\ \vdots & \ddots & \vdots \\ F_{c1}(u) & \cdots & F_{cd}(u) \end{pmatrix}.$$

Notice $F_{ij} : \mathbb{R}^d \times \mathring{K} \to \mathbb{R}$, $i \in I, j \in J$. Denote $F_i(u) = (F_{i1}(u),\cdots,F_{id}(u))^T$, $i \in I$.

3.1 Mass preservation

If $F(u) = (F_1(u),\cdots,F_c(u))^T$, then (6) becomes

$$\begin{pmatrix} u_1 \\ \vdots \\ u_c \end{pmatrix}_t = -\begin{pmatrix} \sum_{j=1}^d (F_{1j})_{x_j} \\ \vdots \\ \sum_{j=1}^d (F_{cj})_{x_j} \end{pmatrix}. \tag{7}$$

If one uses a lexicographic ordering in d-dimensions (the ordering in MATLAB), and U_i stands for U_i at all points in X_C accordingly, then for any fixed $i \in I$, its mimetic scheme can be written as

$$\frac{1}{\Delta t}\left(U_i^{m+1} - U_i^m\right) = -D_{x_1\cdots x_d} I^D_{x_1\cdots x_d} F_i(U^m) = -\sum_{j=1}^d D_{x_1\cdots x_d,j} I^D_{x_1\cdots x_d,j} F_i(U^m), \qquad \forall i \in I.$$

Multiplying by $h\,\mathbb{1}^T$ on the left, one obtains using (5) for Q, that

$$\begin{aligned} h\,\mathbb{1}^T Q(U_i^{m+1} - U_i^m) &= -\Delta t\, h\,\mathbb{1}^T \sum_{j=1}^d Q_{x_1\cdots x_d,j} D_{x_1\cdots x_d,j} I^D_{x_1\cdots x_d,j} F_i(U^m) \\ &= -\Delta t \sum_{l=1}^d (F_{il}(u(x_l^+,t_m)) - F_{il}(u(x_l^-,t_m))), \end{aligned} \tag{8}$$

where $x_l^{\pm} = (x_1,\cdots,x_{l-1},\pm 1,x_{l+1},\cdots,x_d)$. The last identity follows from (5) when $\Delta x_1,\cdots,\Delta x_d \to 0$, and the property that the first and last rows of the identity operators are, respectively, the Kronecker products of $(1,0,\cdots,0)$ and $(0,\cdots,0,1)$ applied to the j-th component and the identity matrix for the other components.

The left hand side of (8) is the difference of discrete mass $\mathcal{M}_i^{m+1}$ of U_i at time t_{m+1} and the discrete mass $\mathcal{M}_i^m$ at time t_m. Therefore, the mass is preserved from time step to time step in the sense that it changes according to the fluxes through all boundaries of $[-1,1]^d$.

3.2 Energy preservation

If one multiplies the i-th equation $i \in I$ of (7) by u_i, and integrates over $L = [-1,1]^d$, one gets

$$\frac{1}{2}\int_L \frac{du_i^2}{dt}\,dx = -\int_L u_i \sum_{j=1}^d (F_{ij}(u))_{x_j}\,dx = \int_L F_i(u)\cdot \mathrm{grad}(u_i)\,dx - \int_L \mathrm{div}(u_i\,F_i)\,dx. \tag{9}$$

If $\mathcal{E}(U_i^l)$ is the discrete energy associated to U_i^l then the discrete analog of (9) is

$$\frac{1}{\Delta t}\left(\mathcal{E}(U_i^{m+1})-\mathcal{E}(U_i^m)\right)=h\,\langle PGU_i, I^D F_i(U)\rangle - h\,\langle QDH_i(U),\mathbb{1}\rangle, \tag{10}$$

with $H_i(U)=I^D(U_i\circ F_i^T(U))$, being $\circ$ the discrete Hadamard product.

From the extended Gauss divergence theorem [10], applied to $F=U_i$ and $\vec{V}=F_i(U)$, one gets that

$$\begin{aligned} h\,\langle PGU_i, I^D F_i(U)\rangle &= U_i^T\bar{B}I^D F_i(U) - h\,\langle D^T Q U_i, I^D F_i^T(U)\rangle \\ &= U_i^T\bar{B}I^D F_i(U) - h\sum_{l\in|X_C|} U_{il}\langle D^T Q\mathbb{1}, I^D F_i^T(U)\rangle, \end{aligned}$$

up to high-order for

$$\bar{B}_{x_1\cdots x_d}=\begin{pmatrix} I_{m_d+2}\otimes\cdots\otimes I_{m_2+2}\otimes\bar{B}_{x_1} & & \\ & \ddots & \\ & & \bar{B}_{x_d}\otimes I_{m_{d-1}+2}\otimes\cdots\otimes I_{m_1+2}\end{pmatrix},$$

where $\bar{B}_p$ is the one dimensional boundary $\bar{B}_{x_p}$ matrix along the p-axis [10]. The second identity comes from the fact that $U_i(x)=\sum_{l\in|X_C|}U_{il}\mathbb{1}(x)$, for $x\in X_C$ and $\mathbb{1}\in\mathbb{R}^{|X_C|\times 1}$, the constant one discrete function.

Therefore, (10) becomes

$$\frac{1}{\Delta t}\left(\mathcal{E}(U_i^{m+1})-\mathcal{E}(U_i^m)\right)=U_i^T\bar{B}I^D F_i(U)-\sum_{l\in|X_C|}U_{il}(h\,\mathbb{1}^T QD)I^D F_i^T(U)-(h\,\mathbb{1}^T QD)H_i(U).$$

Since

$$\begin{aligned} U_i^T\bar{B}I^D F_i(U) &= \sum_{j=1}^{d}[\,U_i(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)I^D F_{ij}(U(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)) \\ &- U_i(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d)I^D F_{ij}(U(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d))\,], \end{aligned}$$

and,

$$\sum_{l\in|X_C|}U_{il}(h\,\mathbb{1}^T QD)I^D F_i^T(U)=\sum_{l\in|X_C|}U_{il}(-1,0,\cdots,0,1)^T I^D F_i^T(U) =$$

$$\sum_{j=1}^{d}[\,U_i(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)I^D F_{ij}(U(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)) - U_i(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d)I^D F_{ij}(U(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d))\,],$$

then, the first two terms cancel out. In addition, since

$$(h\,\mathbb{1}^T QD)H_i(U)=\sum_{j=1}^{d}(H_{ij}(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)-H_{ij}(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d)),$$

then $\mathcal{E}(U_i^{m+1})-\mathcal{E}(U_i^m)=\Delta t(h\,\mathbb{1}^T QD)H_i(U)$ and the difference in energy between two consecutive time steps is the difference in flux across the different boundaries of $[-1,1]^d$, which shows energy preservation of the scheme if one uses the discrete standard energy definition.

3.3 Other quantities preserved for systems of conservation laws

Suppose that each of the components of u, namely u_i, $i \in I$, preserves in time a possibly different quantity v_i, $i \in I$. Assume also that

$$\frac{dv_i}{dt}(u_i) = \frac{dv_i}{du_i}\,\frac{du_i}{dt} = w_i(u_i)\,\frac{du_i}{dt}, \qquad i \in I.$$

For example, for mass preservation is $v_i = u_i, w_i = 1$, and for energy preservation $v_i = \frac{1}{2}u_i^2, w_i = u_i$.

Notice that the quantity $v_i = v_i(u_i)$ could actually depend on all and being of the form $v_i = v(u)$. In that. case, for each $i \in I$,

$$\frac{dv_i}{dt}(u) = \sum_{j=1}^{d} \frac{dv_i}{du_j}\,\frac{du_j}{dt} = \sum_{j=1}^{d} w_{ij}(u)\,\frac{du_j}{dt}.$$

In what follows, by linearity of the derivative in time, it is enough to assume that $v_i = v_i(u_i)$.

Consider $w = (w_1, \cdots, w_c)^T, v = (v_1, \cdots, v_c)^T$.

If one multiplies the i-th equation $i \in I$ of (7) by $w_i(u_i)$, and integrates over $L = [-1,1]^d$, one gets

$$\int_L \frac{dv_i}{dt}(u_i)\,dx = -\int_L w_i(u_i)\sum_{j=1}^{d}(F_{ij}(u))_{x_j}\,dx = \int_L F_i(u)\cdot \mathrm{grad}(w_i(u_i))\,dx - \int_L \mathrm{div}(w_i(u_i)\,F_i)\,dx. \tag{11}$$

If $\mathcal{V}(U_i^l)$ is the discrete preserved quantity associated to U_i^l then the discrete analog of (11) is

$$\frac{1}{\Delta t}\left(\mathcal{V}(U_i^{m+1}) - \mathcal{V}(U_i^m)\right) = h\,\langle PGW_i(U_i), I^D F_i(U)\rangle - h\,\langle QDH_i(U), \mathbb{1}\rangle, \tag{12}$$

with $H_i(U) = I^D(W_i(U_i)\circ F_i^T(U))$, and W_i the projection of w_i onto X_C.

The extended Gauss divergence theorem applied to $F = W_i(U_i)$ and $\vec{V} = F_i(U)$ provides

$$\begin{aligned} h\,\langle PGW_i(U_i), I^D F_i(U)\rangle &= (W_i(U_i))^T \bar{B} I^D F_i(U) - h\,\langle D^T Q W_i(U_i), I^D F_i^T(U)\rangle \\ &= (W_i(U_i))^T \bar{B} I^D F_i(U) - h\sum_{l\in|X_C|} W_i(U_{il})\langle D^T Q\mathbb{1}, I^D F_i^T(U)\rangle. \end{aligned}$$

Therefore, (12) becomes

$$\frac{1}{\Delta t}\left(\mathcal{V}(U_i^{m+1}) - \mathcal{V}(U_i^m)\right) = (W_i(U_i))^T \bar{B} I^D F_i(U) - \sum_{l\in|X_C|} W_i(U_{il})(h\,\mathbb{1}^T QD) I^D F_i^T(U) - (h\,\mathbb{1}^T QD) H_i(U).$$

Since

$$\begin{aligned} (W_i(U_i))^T \bar{B} I^D F_i(U) &= \\ \sum_{j=1}^{d} [\, W_i(U_i(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)) I^D F_{ij}(U(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)) &- \\ (W_i(U_i(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d)) I^D F_{ij}(U(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d))\,], \end{aligned}$$

and,

$$\sum_{l\in|X_C|} W_i(U_{il})(h\,\mathbb{1}^T QD)I^D F_i^T(U) = \sum_{l\in|X_C|} W_i(U_{il})(-1,0,\cdots,0,1)^T I^D F_i^T(U) \quad =$$

$$\sum_{j=1}^{d} [\, W_i(U_i(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d))I^D F_{ij}(U(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d)) \quad -$$

$$W_i(U_i(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d))I^D F_{ij}(U(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d))\,],$$

then, the first two terms cancel out. Furthermore,

$$(h\,\mathbb{1}^T QD)H_i(U) = \sum_{j=1}^{d}(H_{ij}(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d) - H_{ij}(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d)),$$

then $\mathcal{V}(U_i^{m+1}) - \mathcal{V}(U_i^m) = \Delta t(h\,\mathbb{1}^T QD)H_i(U)$ and the difference in $\mathcal{V}$ between two consecutive time steps is the difference in flux across the different boundaries of $[-1,1]^d$, which shows $\mathcal{V}$ preservation of the scheme.

3.4 Quantities preserved for conservation laws in curvilinear structured grids

This section investigates whether or not mimetic schemes preserves quantities for systems of conservation laws given on curvilinear geometries that are defined by structured grids. Here, we distinguish between the physical or curvilinear grid, with x-coordinates, and the logical or computational Cartesian grid, with ξ-coordinates.

Therefore, consider the system of conservation laws given by (6) defined on a curvilinear domain. More specifically, suppose the system of conservation laws is given on a physical spatial domain $\mathcal{P} = \mathcal{X}(L)$ in d-dimensions, with coordinates $x_1,\cdots,x_d$, i.e., $\mathcal{P}$ is the result of a bijective smooth map $\mathcal{X}$ given by

$$x_i = x_i(\xi_1,\cdots,\xi_d), \qquad i\in\{1,\cdots,d\},$$

and that the inverse map of $\mathcal{X}$ is Θ, which is given by

$$\xi_i = \xi(x_1,\cdots,x_d), \qquad i\in\{1,\cdots,d\},$$

and it maps $\mathcal{P}$ onto the logical d-dimensional Cartesian domain $L = [-1,1]^d$. Therefore,

$$\begin{aligned} u_t + \operatorname{div}(F(u)) &= 0_{c\times 1}, & (x,t)\in \mathring{\mathcal{P}}\times\mathring{K}, \\ u(x,0) &= u^0(x), & x\in\mathcal{P}, \end{aligned} \tag{13}$$

and boundary conditions established on $\partial\mathcal{P}$ by

$$\begin{aligned} u_i(\mathcal{X}(x_1,\cdots,x_{j-1},-1,x_{j+1},\cdots,x_d,t)) &= g_i^-(\mathcal{X}(x_1,\cdots,x_{j-1},x_{j+1},\cdots,x_d,t)), \quad i\in I, j\in J, \\ u_i(\mathcal{X}(x_1,\cdots,x_{j-1},1,x_{j+1},\cdots,x_d,t)) &= g_i^+(\mathcal{X}(x_1,\cdots,x_{i-1},x_{i+1},\cdots,x_d,t)), \quad i\in I, j\in J, \end{aligned}$$

where $g_i^\pm : \mathcal{X}(L_0)\times K \to \mathbb{R}^c$, $i = 1,\cdots,c$, are smooth functions. The flux F is defined as before by

$$F(u) = \begin{pmatrix} F_{11}(u) & \cdots & F_{1d}(u) \\ \vdots & \ddots & \vdots \\ F_{c1}(u) & \cdots & F_{cd}(u) \end{pmatrix},$$

where $F_{ij} : \mathbb{R}^d \times \mathring{K} \to \mathbb{R}$, $i \in I, j \in J$, and $F_i(u) = (F_{i1}(u), \cdots, F_{id}(u))^T$, $i \in I$.

If one defines a staggered grid on L, composed of faces X_F and centers (and boundaries) X_C, then $\mathcal{X}(X_C \cup X_F)$ is an structured staggered grid on $\mathcal{P}$, with centers (and boundaries) $\mathcal{C} = \mathcal{X}(X_C)$ and faces $\mathcal{F} = \mathcal{X}(X_F)$.

The Jacobian of the transformation $\mathcal{X}$ is given by

$$J = \frac{\partial(x_1, \cdots, x_d)}{\partial(\xi_1, \cdots, \xi_d)} = \begin{bmatrix} x_{1,\xi_1} & \cdots & x_{1,\xi_d} \\ \vdots & \ddots & \vdots \\ x_{d,\xi_1} & \cdots & x_{d,\xi_d} \end{bmatrix}.$$

For $u : \mathcal{X}(L) \to \mathbb{R}$, with $u = u(x_1, \cdots, x_d) = u(x_1(\xi_1, \cdots, \xi_d), \cdots, x_d(\xi_1, \cdots, \xi_d)) = u(\xi_1, \cdots, \xi_d)$, the chain rule implies

$$u_{\xi_i} = \sum_{j=1}^{d} u_{x_j} x_{j,\xi_i},$$

or equivalently,

$$\begin{bmatrix} u_{\xi_1} \\ \vdots \\ u_{\xi_d} \end{bmatrix} = \begin{bmatrix} x_{1,\xi_1} & \cdots & x_{d,\xi_1} \\ \vdots & \ddots & \vdots \\ x_{1,\xi_d} & \cdots & x_{d,\xi_d} \end{bmatrix} \begin{bmatrix} u_{x_1} \\ \vdots \\ u_{x_d} \end{bmatrix} = J^T \begin{bmatrix} u_{x_1} \\ \vdots \\ u_{x_d} \end{bmatrix}.$$

Hence

$$\begin{bmatrix} u_{x_1} \\ \vdots \\ u_{x_d} \end{bmatrix} = (J^T)^{-1} \begin{bmatrix} u_{\xi_1} \\ \vdots \\ u_{\xi_d} \end{bmatrix}.$$

If one uses the gradient to approximate the partial derivatives of the Jacobian, then

$$J_G^T = I^G_{x_1 \cdots x_d} \tilde{G}_{\xi_1 \cdots \xi_d},$$

where $\tilde{G}_{x_1 \cdots x_d}$ is $G_{x_1 \cdots x_d}$ with $\hat{I}_p$ replaced by I_{p+2}, the identity matrix of order $p + 2$ (see [10]).

If one computes the Jacobian at the faces then the physical gradient is given by

$$G_{x_1 \cdots x_d} = (J_G^T)^{-1} G_{\xi_1 \cdots \xi_d}.$$

Similarly, one can construct the Jacobian (at the centers) based on the divergence operator.

The extended Gauss divergence theorem in the physical domain should read

$$h \langle G_{x_1 \cdots x_d} F(x), \vec{V}(x) \rangle_{P_{x_1 \cdots x_d}} + h \langle D_{x_1 \cdots x_d} \vec{V}(x), F(x) \rangle_{Q_{x_1 \cdots x_d}} = F^T(x) \bar{B}_{x_1 \cdots x_d} \vec{V}(x),$$

and hence

$$h \langle (J_G^T)^{-1} G_{\xi_1 \cdots \xi_d} F(\xi), \vec{V}(\xi) \rangle_{P_{x_1 \cdots x_d}} + h \langle (J_D^T)^{-1} D_{\xi_1 \cdots \xi_d} \vec{V}(\xi), F(\xi) \rangle_{Q_{x_1 \cdots x_d}} = F^T(\xi) \bar{B}_{\xi_1 \cdots \xi_d} \vec{V}(\xi),$$

or equivalently,

$$h \langle G_{\xi_1 \cdots \xi_d} F(\xi), \vec{V}(\xi) \rangle_{P_{x_1 \cdots x_d} (J_G^T)^{-1}} + h \langle D_{\xi_1 \cdots \xi_d} \vec{V}(\xi), F(\xi) \rangle_{Q_{x_1 \cdots x_d} (J_D^T)^{-1}} = F^T(\xi) \bar{B}_{\xi_1 \cdots \xi_d} \vec{V}(\xi),$$

which conserves the identity for

$$Q_{x_1\cdots x_d} = Q_{\xi_1\cdots\xi_d} J_D^T, \qquad P_{x_1\cdots x_d} = P_{\xi_1\cdots\xi_d} J_G^T,$$

since the Dirichlet boundary condition $\bar{B}_{\xi_1\cdots\xi_d} = \bar{B}_{x_1\cdots x_d}$ does not change.

For constant scalar field $F(\xi)$, one gets $h\,\langle D_{\xi_1\cdots\xi_d}\vec{V}(\xi), \mathbb{1}\rangle_{Q_{\xi_1\cdots\xi_d}} = \mathbb{1}^T \bar{B}_{\xi_1\cdots\xi_d}\vec{V}(\xi)$, which implies that $\mathbb{1}^T\bar{B}_{\xi_1\cdots\xi_d} = h\,\mathbb{1}^T Q_{\xi_1\cdots\xi_d} D_{\xi_1\cdots\xi_d} = h\,\mathbb{1}^T(Q_{\xi_1\cdots\xi_d}J_D^T)((J_D^T)^{-1}D_{\xi_1\cdots\xi_d})$, and hence

$$h\,\mathbb{1}^T Q_{x_1\cdots x_d} D_{x_1\cdots x_d} = \mathbb{1}^T \bar{B}_{x_1\cdots x_d}.$$

Similarly, for constant vector field $\vec{V}(\xi)$, one gets

$$h\,\mathbb{1}^T P_{x_1\cdots x_d} G_{x_1\cdots x_d} = \mathbb{1}^T \bar{B}^T_{x_1\cdots x_d}.$$

Suppose that each of the components of u, namely u_i, $i \in I$, preserves in time a possibly different quantity v_i, $i \in I$. Assume also that

$$\frac{dv_i}{dt}(u_i(x)) = \frac{dv_i}{du_i}(u_i(\xi))\,\frac{du_i}{dt}(\xi) = z_i(u_i(\xi))\,\frac{du_i(\xi)}{dt} = \frac{w_i}{|J|}(u_i(\xi))\,\frac{du_i}{dt}(\xi), \qquad i \in I,$$

where $|J|$ is the Jacobian determinant. Consider $w = (w_1, \cdots, w_c)^T, v = (v_1, \cdots, v_c)^T$.

If one multiplies the i-th equation $i \in I$ of (13) by $z_i(u_i(\xi(x)))$, and integrates over $\mathcal{P}$, one gets

$$\begin{aligned}\int_{\mathcal{P}} \frac{dv_i}{dt}(u_i(x))\,dx &= -\int_{\mathcal{P}} z_i(u_i(x))\,\sum_{j=1}^{d}(F_{ij}(u(x)))_{x_j}\,dx \\ &= \int_{\mathcal{P}} F_i(u(x))\cdot G_{x_1\cdots x_d}(z_i(u_i(x)))\,dx - \int_{\mathcal{P}} D_{x_1\cdots x_d}(z_i(u_i(x))\,F_i(u(x)))\,dx.\end{aligned}$$

The change of variable for multiple integral allows to write the previous identity as

$$\int_{\mathcal{P}} \frac{dv_i}{dt}(u_i(\xi))\,dx = \int_L F_i(u(\xi))\cdot(J_G^T)^{-1}G_{\xi_1\cdots\xi_d}(w_i(u_i(\xi)))\,d\xi - \int_L (J_D^T)^{-1}D_{\xi_1\cdots\xi_d}(w_i(u_i(\xi))\,F_i(u(\xi)))\,d\xi,$$

If $\mathcal{K}(U_i^l)$ is the discrete preserved quantity associated to U_i^l, then the discrete analog of the previous identity is

$$\frac{1}{\Delta t}\,(\mathcal{K}(U_i^{m+1}) - \mathcal{K}(U_i^m)) = h\,\langle P_{\xi_1\cdots\xi_d}G_{\xi_1\cdots\xi_d}W_i(U_i), I^D F_i(U)\rangle - h\,\langle Q_{\xi_1\cdots\xi_d}D_{\xi_1\cdots\xi_d}H_i(U), \mathbb{1}\rangle, \quad (14)$$

with $H_i(U) = I^D(W_i(U_i) \circ F_i^T(U))$.

The extended Gauss divergence theorem applied to $F = W_i(U_i)$ and $\vec{V} = F_i(U)$ provides

$$\begin{aligned}h\,\langle P_{\xi_1\cdots\xi_d}G_{\xi_1\cdots\xi_d}W_i(U_i), I^D F_i(U)\rangle &= (W_i(U_i))^T\bar{B}_{\xi_1\cdots\xi_d}I^D F_i(U) - h\,\langle D^T_{\xi_1\cdots\xi_d}Q_{\xi_1\cdots\xi_d}W_i(U_i), I^D F_i^T(U)\rangle \\ &= (W_i(U_i))^T\bar{B}_{\xi_1\cdots\xi_d}I^D F_i(U) - h\sum_{l\in|X_C|} W_i(U_{il})\langle D^T_{\xi_1\cdots\xi_d}Q_{\xi_1\cdots\xi_d}\mathbb{1}, I^D F_i^T(U)\rangle.\end{aligned}$$

Similar identities like the ones utilized for the quantities preserved for the non-curvilinear case demonstrate that $\mathcal{K}(U_i^{m+1}) - \mathcal{K}(U_i^m) = \Delta t\,(h\,\mathbb{1}^T Q_{\xi_1\cdots\xi_d}D_{\xi_1\cdots\xi_d})H_i(U)$. Hence, the difference in $\mathcal{K}$ between two consecutive time steps is the difference in flux across the different boundaries of $[-1,1]^d$, which shows $\mathcal{K}$ preservation of the scheme.

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