

CHAPTER 1

CURVILINEAR GRIDS

1.1. TRANSFORMATION OF CONSERVATION LAW

We are working with the conservation law

$$\mathbf{u}_t + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) = \mathbf{0}$$

on a domain Ω which is partitioned into M non-overlapping quadrilateral elements Ω_e which can be deformed or curved

$$\Omega = \bigcup_{e=1}^M \Omega_e. \quad (1.1)$$

Each quadrilateral element can be mapped into a reference quadrilateral $\Omega_s = [0, 1]^3$ in the transformed space

$$\boldsymbol{\xi} = (\xi, \eta, \zeta) = (\xi_1, \xi_2, \xi_3),$$

with the generic mapping

$$\mathbf{x} = \Theta_e(\boldsymbol{\xi}), \quad (1.2)$$

where the e would usually be suppressed. For an arbitrary shaped element, the mapping would look like

$$\Theta(\boldsymbol{\xi}) = \sum_{p,q,r=0}^P \hat{\mathbf{x}}_{p,q,r} \phi_{pqr}(\boldsymbol{\xi}), \quad (1.3)$$

where $\{\phi_{pqr}\}$ is the Lagrange basis corresponding to the points $\{\hat{\mathbf{x}}_{p,q,r}\}$, explicitly written in terms of tensor product polynomials

$$\phi_{pqr}(\boldsymbol{\xi}) = \phi_p(\xi_1) \phi_q(\xi_2) \phi_r(\xi_3).$$

That is, the mapping is a degree P polynomial in each direction.

We define the covariant and contravariant basis

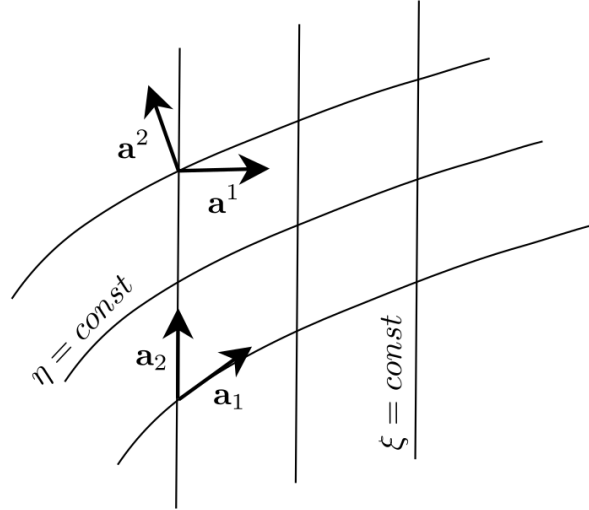


Figure 1.1. Covariant and contravariant coordinate vectors in relation to the coordinate lines

DEFINITION 1.1. *Covariant basis*

The covariant basis \mathbf{a}_i , $i = 1, 2, 3$, varies along a coordinate line. It is the tangent to the coordinate line

$$\mathbf{a}_i = \lim_{\Delta \xi^i \rightarrow 0} \frac{\Delta \mathbf{x}}{\Delta \xi^i} = \frac{\partial \mathbf{x}}{\partial \xi^i}, \quad i = 1, 2, 3. \quad (1.4)$$

Covariant basis vectors are the vectors that we can actually compute from the mapping function $\mathbf{x}(\xi)$.

By its definition, covariant basis vector \mathbf{a}_i is tangent to the curve where \mathbf{x} varies along ξ_i .

Remark 1.2. Here we prove that $\mathbf{a}_1, \mathbf{a}_2$ will be tangent to the coordinate line $\xi_3 = \xi_{30}$. For any point $\mathbf{X}^0 = \mathbf{x}(\xi_{10}, \xi_{20}, \xi_{30}) = \Theta(\xi_{10}, \xi_{20}, \xi_{30})$ on $\xi_3 = \xi_{30}$, we can find curves

$$\begin{aligned} \mathbf{X}^1(t) &= \mathbf{x}(\xi_{10} + t, \xi_{20}, \xi_{30}) = \Theta(\xi_{10} + t, \xi_{20}, \xi_{30}), \\ \mathbf{X}^2(t) &= \mathbf{x}(\xi_{10}, \xi_{20} + t, \xi_{30}) = \Theta(\xi_{10}, \xi_{20} + t, \xi_{30}), \end{aligned}$$

which lie on $\xi_3 = \xi_{30}$. Thus, the tangent vectors of $\xi_3 = \text{const}$ are clearly given by

$$\left. \frac{\partial \mathbf{x}}{\partial \xi_1} \right|_{\mathbf{x}=\mathbf{X}^0}, \quad \left. \frac{\partial \mathbf{x}}{\partial \xi_2} \right|_{\mathbf{x}=\mathbf{X}^0}.$$

DEFINITION 1.3. *Contravariant basis*

The contravariant basis vectors are normal to the **coordinate lines** and are defined by the gradients

$$\mathbf{a}^i = \nabla_{\mathbf{x}} \xi^i \quad i = 1, 2, 3. \quad (1.5)$$

Formally, it appears that we need the inverse transformation $\boldsymbol{\xi} = \mathbf{X}^{-1}(\mathbf{x})$ to compute the contravariant basis vectors.

Remark 1.4. We will later prove that

$$\mathbf{x}_i \times \mathbf{x}_j = J \nabla_{\mathbf{x}} \xi^k,$$

which will show that $\mathbf{a}^k = \nabla_{\mathbf{x}} \xi^k$ is perpendicular to $\mathbf{x}_i, \mathbf{x}_j$ which are the tangent vectors on $\xi_3 = \text{const}$, as proven in the previous remark.

The first step to transforming equations is to write how derivative operators transform under a mapping. First, we see that we can write a differential element in terms of the covariant basis vectors

$$d\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \xi} d\xi + \frac{\partial \mathbf{x}}{\partial \eta} d\eta + \frac{\partial \mathbf{x}}{\partial \zeta} d\zeta = \sum_{i=1}^3 \mathbf{a}_i d\xi^i. \quad (1.6)$$

The arc length is the magnitude of this vector

$$(ds)^2 = |d\mathbf{x}|^2 = \sum_{i=1}^3 \sum_{j=1}^3 \mathbf{a}_i \cdot \mathbf{a}_j d\xi^i d\xi^j = \sum_{i=1}^3 \sum_{j=1}^3 g_{ij} d\xi^i d\xi^j, \quad (1.7)$$

where we have used the definition of the *covariant metric tensor* $g_{ij} \equiv \mathbf{a}_i \cdot \mathbf{a}_j = g_{ji}$ to simplify the sums.

Next, we define the surface area element, which we compute from the cross product (Fig. 1.2)

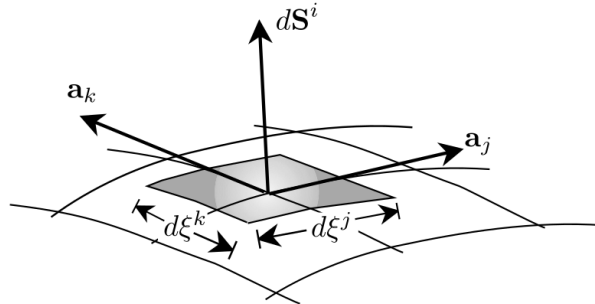


Figure 1.2. Surface element vector computed from covariant basis vectors

$$d\mathbf{S}^i = \mathbf{a}_j d\xi^j \times \mathbf{a}_k d\xi^k = (\mathbf{a}_j \times \mathbf{a}_k) d\xi^j d\xi^k. \quad (1.8)$$

Here, i, j, k are considered to be *cyclic*, so knowing one will fix the rest. Thus, a surface element in Cartesian space with size Δx in the \hat{x} direction and Δy in \hat{y} direction has the surface element

$$dS^{(z)} = \Delta x \Delta y \hat{z}$$

according to this relation.

Finally the volume element extends the surface element in normal direction

$$dV = \mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k) d\xi^i d\xi^j d\xi^k. \quad (1.9)$$

We know that

$$\mathbf{a}_i \cdot (\mathbf{a}_j \times \mathbf{a}_k) = \sqrt{\det(g)} =: J, \quad (1.10)$$

giving the well-known result from calculus

$$dV = J d\xi^i d\xi^j d\xi^k. \quad (1.11)$$

We can now derive how different derivative operators transform under the mapping. First, recall that the divergence of a flux, \mathbf{F} , is defined as

$$\nabla \cdot \mathbf{F} = \lim_{\Delta V \rightarrow 0} \frac{1}{\Delta V} \int_{\partial \Delta V} \mathbf{F} \cdot d\mathbf{S}. \quad (1.12)$$

If we take the volume to be a differential pillbox, see Fig. 1.3, the surface integral can be broken into

$$\sum_{i=1}^3 \{F \cdot (a_j \times a_k) \Delta \xi^j \Delta \xi^k |^+ - F \cdot (a_j \times a_k) \Delta \xi^j \Delta \xi^k |^-\}. \quad (1.13)$$

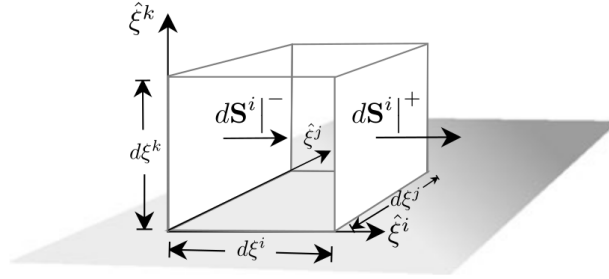


Figure 1.3. Differential volume element for divergence

With $\Delta V = J \Delta \xi^i \Delta \xi^j \Delta \xi^k$,

$$\frac{1}{\Delta V} \int_{\partial V} \mathbf{F} \cdot d\mathbf{S} = \frac{1}{J} \sum_{i=1}^3 \left\{ \frac{F \cdot (a_j \times a_k) \Delta \xi^j \Delta \xi^k |^+ - F \cdot (a_j \times a_k) \Delta \xi^j \Delta \xi^k |^-}{\Delta \xi^i \Delta \xi^j \Delta \xi^k} \right\}. \quad (1.14)$$

The limit as $\Delta V \rightarrow 0$ gives the divergence,

$$\nabla \cdot \mathbf{F}(\mathbf{x}) = \frac{1}{J} \sum_{i=1}^3 \frac{\partial}{\partial \xi^i} (F \cdot (a_j \times a_k))(\boldsymbol{\xi}). \quad (1.15)$$

This is known as the *conservative form* of the divergence because of its relation to the differential form of a conservation law.

We derive an alternative, called *non-conservative form*, by noting that the divergence is invariant under the transformation. Suppose that $\mathbf{F} = \mathbf{c}$, then

$$\nabla \cdot \mathbf{F} = \frac{1}{J} \sum_{i=1}^3 \frac{\partial}{\partial \xi^i} (c \cdot (a_j \times a_k)) = 0. \quad (1.16)$$

Since \mathbf{c} is arbitrary, we must have

$$\sum_{i=1}^3 \frac{\partial}{\partial \xi^i} (a_j \times a_k) = \mathbf{0}. \quad (1.17)$$

We are just using $\mathbf{c} \cdot \mathbf{v} = 0$ for all \mathbf{c} implies $\mathbf{v} \equiv 0$. These (1.17) are known as *metric identities* (plural because it's a vector equation). The metric identities primarily say that the **divergence in computational space of specific products of the covariant basis must vanish**.

Using the metric identities, we rewrite the divergence (1.15) in non-conservative form

$$\nabla \cdot \mathbf{F} = \frac{1}{J} \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot \frac{\partial \mathbf{F}}{\partial \xi^i}. \quad (1.18)$$

We now use the representation of divergence operator to **write the representation of gradient operator in computational space**. If we write out the terms in nonconservative form of the divergence, we get

$$\frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z} = \nabla \cdot \mathbf{F} = \frac{1}{J} \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot \left(\frac{\partial F_1}{\partial \xi^i} \hat{x} + \frac{\partial F_2}{\partial \xi^i} \hat{y} + \frac{\partial F_3}{\partial \xi^i} \hat{z} \right).$$

Matching the terms on either side, we will get, for a scalar, f ,

$$\nabla f = \frac{1}{J} \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \frac{\partial f}{\partial \xi^i}. \quad (1.19)$$

We use the conservative identities, (1.17) again, to derive the conservative form

$$\nabla f = \frac{1}{J} \sum_{i=1}^3 \frac{\partial}{\partial \xi^i} [(\mathbf{a}_j \times \mathbf{a}_k) f]. \quad (1.20)$$

Note that all the transformations of the differential operators are in terms of quantities that we can compute directly from the mapping, namely the covariant basis vectors, \mathbf{a}_i .

We use the gradient relations to find the contravariant basis vectors. To relate the contravariant and covariant basis vectors, we set $f = \xi^i$ in (1.20). Then, the gradient of ξ^i is

$$\nabla_{\mathbf{x}} \xi^i = \frac{1}{J} \sum_{l=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \frac{\partial \xi^i}{\partial \xi^l}, \quad (1.21)$$

with (l, j, k) cyclic. Since $\partial \xi^i / \partial \xi^l = \delta_{i,l}$,

$$\nabla \xi^i = \mathbf{a}^i = \frac{1}{J} (\mathbf{a}_j \times \mathbf{a}_k), \quad (1.22)$$

or

$$J \mathbf{a}^i = \mathbf{a}_j \times \mathbf{a}_k. \quad (1.23)$$

Recall that our transformations from computational to physical domains are constructed so that physical boundaries correspond to either a $\xi = \text{const}$ or $\eta = \text{const}$ line, we can compute boundary normals from the contravariant basis vectors. Boundary normals are needed to set Neumann or normal flux boundary conditions. Since the contravariant basis vectors are normal to a coordinate line, a normal in the positive direction of the i^{th} coordinate variable is in the direction of \mathbf{a}^i . Thus, we have a normal in direction of increasing ξ^i to be

$$\hat{n}^i = \frac{|J|}{J} \frac{\mathbf{a}_j \times \mathbf{a}_k}{\|\mathbf{a}_j \times \mathbf{a}_k\|}, \quad (1.24)$$

where $\|\cdot\|$ denotes the Euclidean norm of the vector. Here i corresponds to the i^{th} direction boundary normals in reference coordinates.

The relationship between the covariant and contravariant basis vectors

$$J \mathbf{a}^i = \mathbf{a}_j \times \mathbf{a}_k,$$

allows us to rewrite the conservative forms of the differential operators that we have derived so far. We can write the divergence in the more compact form

$$\nabla \cdot \mathbf{F} = \frac{1}{J} \sum_{i=1}^3 \frac{\partial}{\partial \xi^i} (J \mathbf{a}^i \cdot \mathbf{F}). \quad (1.25)$$

Similarly, the gradient becomes

$$\nabla f = \frac{1}{J} \sum_{i=1}^3 J \mathbf{a}^i \frac{\partial f}{\partial \xi^i}. \quad (1.26)$$

Finally, the metric identities (1.17) are equivalent to

$$\sum_{i=1}^3 \frac{\partial J \mathbf{a}^i}{\partial \xi^i} = \mathbf{0}. \quad (1.27)$$

We explain the construction of grid and its reference maps to master cube $[0, 1]^3$ in Section 1.2. Within each element Ω_e , we obtain the transformed conservation law

$$\tilde{\mathbf{u}}_t + \nabla \cdot \tilde{\mathbf{f}} = 0, \quad (1.28)$$

where

$$\begin{aligned} \tilde{\mathbf{u}} &= J \vec{Q}, \\ \tilde{\mathbf{f}}^i &= J \vec{a}^i \cdot \vec{F} = \sum_{n=1}^3 J a_n^i \vec{F}_n. \end{aligned} \quad (1.29)$$

1.2. CREATION AND STORAGE OF GRIDS

1. Structured Grids

One master map from $[-1, 1]^2$ to Ω to form the grid. The structure of code is

```
calc_volume_integral! # Element loop where values Ub, Fb extrapolated to face
calc_interface_flux!  # Element loop, all numerical fluxes computed
calc_surface_integral! # Element loop, numerical flux contribution added
```

2. Unstructured grids

```
calc_volume_integral! # Element loop. Store Ub, Fb pointwise
prolong_to_interfaces! # Face loop to prolong above computed Ub, Fb
calc_interface_flux!  # Face loop to use prolonged fluxes for numerical flux
calc_surface_integral! # Element loop, numerical flux contribution added
```

1.3. CONSERVATIVE LAX-WENDROFF FLUX RECONSTRUCTION (LWFR) ON CURVILINEAR GRIDS

1.3.1. Discontinuous Galerkin

Use the I_N notation!!

We define degree N Lagrange polynomial basis $\{\ell_{ijk}\}$ on the reference cell $\Omega_s = [0, 1]^3$. Let \mathbf{u}^δ , \mathbf{f}^δ be the approximate solution and flux in the physical space, which need not be polynomials. Corresponding to each Ω_e , we define as reference map

$$\Theta_e: \Omega_s \rightarrow \Omega_e,$$

using which, we can define degree N approximate solution and flux in the reference space

$$\begin{aligned} \hat{\mathbf{u}}_e^\delta(\boldsymbol{\xi}) &= \sum_{i,j,k=1}^{N+1} \hat{\mathbf{u}}_{e,ijk} \ell_{ijk}(\boldsymbol{\xi}), \\ \hat{\mathbf{f}}_e^\delta(\boldsymbol{\xi}) &= \sum_{i,j,k=1}^{N+1} \mathbf{f}(\hat{\mathbf{u}}_{e,ijk}) \ell_{ijk}(\boldsymbol{\xi}), \end{aligned} \quad (1.30)$$

where $\hat{\mathbf{u}}_{e,ijk}$ are the unknowns we solve for.

We can either formulate the DG scheme for the transformed PDE

$$\mathbf{u}_t + \frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}} = 0, \quad (1.31)$$

where

$$\tilde{\mathbf{f}}^i = J \vec{a}^i \cdot \vec{F} = \sum_{n=1}^3 J a_n^i \vec{F}_n, \quad (1.32)$$

or we can transform the weak formulation. We compare the difference between the two. With that said, we derive the DG scheme for the tranformed conservation law. After change of variables of integration, we will have

$$\int_{\Omega_s} \frac{\partial \mathbf{u}_e^\delta}{\partial t} \varphi(\boldsymbol{\xi}) J d\boldsymbol{\xi} + \int_{\Omega_s} \frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}_e^\delta J d\boldsymbol{\xi} = 0,$$

on which we perform integration by parts to get

$$\int_{\Omega_s} \frac{\partial \mathbf{u}_e^\delta}{\partial t} \varphi(\boldsymbol{\xi}) J d\boldsymbol{\xi} - \int_{\Omega_s} \tilde{\mathbf{f}}_e^\delta \cdot (\nabla_{\boldsymbol{\xi}} \varphi) d\boldsymbol{\xi} + \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} (\tilde{\mathbf{f}}_e^\delta \cdot \mathbf{n}_{s,i})^* \varphi dS_{\boldsymbol{\xi}} = 0,$$

(s, i) corresponds to the two faces in i^{th} direction, $\mathbf{n}_{s,i}$ is the outward unit normal in the reference cell. Let us now start with the DG scheme in the physical cell

$$\int_{\Omega_e} \frac{\partial \mathbf{u}_e^\delta}{\partial t} \varphi(\boldsymbol{\xi}) d\mathbf{x} - \int_{\Omega_e} \mathbf{f}_e^\delta \cdot (\nabla_{\mathbf{x}} \varphi) d\mathbf{x} + \sum_{i=1}^3 \int_{\partial\Omega_{e,i}} (\mathbf{f}_e^\delta \cdot \mathbf{n}_i)^* \varphi dS_{\mathbf{x}} = 0,$$

where (e, i) corresponds to the image of the two faces in i^{th} direction, under the reference map, \mathbf{n}_i is the outward unit normal.

Note that the test functions are still the basis functions in reference cell. The volume and surface change of variables are (1.11, 1.8)

$$\begin{aligned} d\mathbf{x} &= J d\boldsymbol{\xi}, \\ dS_{\mathbf{x}}^i &= \|J \mathbf{a}^i\| dS_{\boldsymbol{\xi}}, \end{aligned}$$

where i indicates the two faces of Ω_e mapped by the i direction faces of Ω_s under Θ_e

The transformations of gradient and normal are (1.26, 1.24)

$$\begin{aligned} \nabla_{\mathbf{x}} \varphi &= \sum_{i=1}^3 \mathbf{a}^i \frac{\partial \varphi}{\partial \xi^i}, \\ \hat{\mathbf{n}}^i &= \frac{\mathbf{a}^i}{\|\mathbf{a}^i\|}. \end{aligned}$$

Thus, performing a change of variables to map to Ω_s , we get

$$\int_{\Omega_s} \frac{\partial \mathbf{u}_e^\delta}{\partial t} \varphi(\boldsymbol{\xi}) J d\boldsymbol{\xi} - \int_{\Omega_s} \mathbf{f}_e^\delta \cdot \left(\sum_{i=1}^3 \mathbf{a}^i \frac{\partial \varphi}{\partial \xi^i} \right) J d\boldsymbol{\xi} + \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} (\mathbf{f}_e^\delta \cdot \mathbf{n}_i)^* \varphi \|J \mathbf{a}^i\| dS_{\boldsymbol{\xi}} = 0.$$

Now,

$$\begin{aligned} \mathbf{f} \cdot \left(\sum_{i=1}^3 \mathbf{a}^i \frac{\partial \varphi}{\partial \xi^i} \right) &= \sum_{n=1}^3 \mathbf{f}_n \cdot \left(\sum_{i=1}^3 a_n^i \frac{\partial \varphi}{\partial \xi^i} \right) J \\ &= \sum_{i=1}^3 \left(\sum_{n=1}^3 J a_n^i \mathbf{f}_n \right) \frac{\partial \varphi}{\partial \xi^i} \\ &= \sum_{i=1}^3 (J \vec{a}^i \cdot \vec{F}) (\nabla_{\boldsymbol{\xi}} \varphi)_i \\ &= \tilde{\mathbf{f}} \cdot (\nabla_{\boldsymbol{\xi}} \varphi) \end{aligned}$$

Thus, the volume terms match. We now compare the surface terms. That is, we compare

$$(\mathbf{f}_e \cdot \mathbf{n}_i)^* \|J \mathbf{a}^i\|$$

and

$$(\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^*$$

on a face. Now,

$$\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i} = \vec{F} \cdot J \vec{d}^i = \|J \mathbf{a}^i\| \vec{F} \cdot \mathbf{n}_i.$$

Thus,

$$(\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* = (\mathbf{f}_e \cdot \mathbf{n}_i)^* \|J \mathbf{a}^i\|,$$

and we get our claim that the two approaches are equivalent.

1.3.2. Flux Reconstruction

We derive the Flux Reconstruction directly from the DG scheme. We take the test function to be

$$\ell_{p_1 p_2 p_3}(\boldsymbol{\xi}) = \ell_{p_1}(\xi^1) \ell_{p_2}(\xi^2) \ell_{p_3}(\xi^3).$$

Replace the $p_1 p_2 p_3$ by \mathbf{p} . The DG scheme in reference cell is given by

$$\begin{aligned} & \int_{\Omega_s} \frac{\partial \mathbf{u}_e^\delta}{\partial t} \ell_{p_1 p_2 p_3} J d\boldsymbol{\xi} - \int_{\Omega_s} \tilde{\mathbf{f}}_e \cdot (\nabla_{\boldsymbol{\xi}} \ell_{p_1 p_2 p_3}) d\boldsymbol{\xi} \\ & + \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} (\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* \ell_{p_1 p_2 p_3} dS_{\boldsymbol{\xi}} \\ & - \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} (\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* \ell_{p_1 p_2 p_3} dS_{\boldsymbol{\xi}} = \mathbf{0}, \end{aligned}$$

where we have made $\mathbf{n}_{s,i}$ independent of face by fixing to be pointed towards the direction where i^{th} coordinate is one, i.e., $\mathbf{n}_{s,i} = \mathbf{e}_i$. We have also used

$$(\tilde{\mathbf{f}}_e \cdot (-\mathbf{n}_{s,i}))^* = -(\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^*.$$

It is trivial for the central part. For the dissipative part, it means that the left and right states have been swapped and wave speed is invariant.

We can perform integration by parts if we use Gauss-Legendre quadrature points (integrals will be exact) or Gauss-Lobatto quadrature points (integrals will be exact along the relevant direction). Thus, the scheme is equivalent to

$$\begin{aligned} & \int_{\Omega_s} \frac{\partial \mathbf{u}_e^\delta}{\partial t} \ell_{p_1 p_2 p_3} d\boldsymbol{\xi} + \frac{1}{J} \int_{\Omega_s} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}_e \ell_{p_1 p_2 p_3} d\boldsymbol{\xi} \\ & + \frac{1}{J} \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i}) \ell_{p_1 p_2 p_3} dS_{\boldsymbol{\xi}} \\ & - \frac{1}{J} \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i}) \ell_{p_1 p_2 p_3} dS_{\boldsymbol{\xi}} = \mathbf{0} \end{aligned}$$

Now, we collocate the scheme at $\{\boldsymbol{\xi}_{p_1 p_2 p_3}\}_{p_1, p_2, p_3=1}^{N+1}$ and use the following notations for a fixed $\boldsymbol{\xi}_{p_1 p_2 p_3}$

$$\begin{aligned} \mathbf{w} &= w_{p_1} w_{p_2} w_{p_3}, & \mathbf{w}_i &= \mathbf{w} / w_{p_i}, \\ \ell &= \ell_{p_1 p_2 p_3}, & \ell_i(\boldsymbol{\xi}) &= \ell_{p_j}(\xi^j) \ell_{p_k}(\xi^k), \quad i, j, k \text{ are in a cycle,} \\ \boldsymbol{\xi}_i^{L/R} & \text{ is the point that agrees with } \boldsymbol{\xi} \text{ at } j, k \text{ and equals 0 or 1 for } L \text{ or } R \text{ at } i. \end{aligned}$$

Performing quadrature at solution points, the collocation scheme at the fixed $\boldsymbol{\xi}_{p_1 p_2 p_3}$ would be

$$\begin{aligned} & \frac{d\mathbf{u}_{e, p_1 p_2 p_3}^\delta}{dt} \mathbf{w} + \frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}_e(\boldsymbol{\xi}_{p_1 p_2 p_3}) \mathbf{w} \\ & + \frac{1}{J} \sum_{i=1}^3 ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^R) \ell_{p_i}(1) \mathbf{w}_i \\ & - \frac{1}{J} \sum_{i=1}^3 ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^L) \ell_{p_i}(0) \mathbf{w}_i = \mathbf{0}. \end{aligned}$$

Dividing by w

$$\begin{aligned} & \frac{d\mathbf{u}_{e,p_1p_2p_3}^\delta}{dt} + \frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}_e(\boldsymbol{\xi}_{p_1p_2p_3}) \\ & + \frac{1}{J} \sum_{i=1}^3 ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^R) \frac{\ell_{p_i}(1)}{w_{p_i}} \\ & - \frac{1}{J} \sum_{i=1}^3 ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^L) \frac{\ell_{p_i}(0)}{w_{p_i}} = 0. \end{aligned}$$

Then, using

$$\frac{\ell_{p_i}(0)}{w_{p_i}}, \frac{\ell_{p_i}(1)}{w_{p_i}} = \begin{cases} -g'_{\text{Radau},L}(\xi_{p_i}), g'_{\text{Radau},R}(\xi_{p_i}), & \text{GL solution points and quadrature,} \\ -g'_{\text{Hu},L}(\xi_{p_i}), g'_{\text{Hu},R}(\xi_{p_i}), & \text{GLL solution points and quadrature,} \end{cases}$$

we obtain

$$\begin{aligned} & \frac{d\mathbf{u}_{e,p_1p_2p_3}^\delta}{dt} + \frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}_e(\boldsymbol{\xi}_{p_1p_2p_3}) \\ & + \frac{1}{J} \sum_{i=1}^3 ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^R) g'_R(\xi_{p_i}) \\ & + \frac{1}{J} \sum_{i=1}^3 ((\tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{f}}_e \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^L) g'_L(\xi_{p_i}) = 0. \end{aligned} \quad (1.33)$$

1.3.2.1. Implementation of cell residual

Cell residual can be computed by the usual D1 matrix, replacing \mathbf{f} by $\tilde{\mathbf{f}}$

1.3.2.2. Implementation of face residual

1.3.3. Lax-Wendroff Flux Reconstruction (LWFR)

We perform the Lax-Wendroff procedure on the equation

$$\mathbf{u}_t + \frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}} = 0, \quad (1.34)$$

where

$$\tilde{\mathbf{f}}^i = J \tilde{\mathbf{a}}^i \cdot \vec{F} = \sum_{n=1}^3 J a_n^i \vec{F}_n. \quad (1.35)$$

We will discretize in time and do a polynomial approximation in space. For a degree N approximation, we will use the update

$$u^{n+1}(\boldsymbol{\xi}) = u^n(\boldsymbol{\xi}) + \sum_{k=1}^N \frac{\Delta t^k}{k!} \partial_t^{(k)} u^n(\boldsymbol{\xi}).$$

Using the transformed PDE (1.34), we get

$$u^{n+1}(\boldsymbol{\xi}) = u^n(\boldsymbol{\xi}) - \frac{1}{J} \sum_{k=1}^N \frac{\Delta t^k}{k!} \partial_t^{(k-1)} (\nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}).$$

Shifting indices and writing in conservative form, we get

$$\mathbf{u}^{n+1}(\boldsymbol{\xi}) = \mathbf{u}^n(\boldsymbol{\xi}) - \frac{\Delta t}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{F}},$$

where

$$\tilde{\mathbf{F}} = \sum_{k=0}^N \frac{\Delta t^k}{(k+1)!} \partial_t^k \tilde{\mathbf{f}}.$$

We will find a local order $N + 1$ approximation $\tilde{\mathbf{F}}_e^\delta$ to $\tilde{\mathbf{F}}$ and then, following (1.33), the LWFR update would be

$$\begin{aligned} & \mathbf{u}^{n+1} - \mathbf{u}^n + \frac{1}{J} \Delta t \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{F}}_e^\delta(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ & + \frac{1}{J} \Delta t \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} ((\tilde{\mathbf{F}}_e^\delta \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{F}}_e^\delta \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^R) g'_R(\xi_{p_i}) dS_{\boldsymbol{\xi}} \\ & + \frac{1}{J} \Delta t \sum_{i=1}^3 \int_{\partial\Omega_{s,i}} ((\tilde{\mathbf{F}}_e^\delta \cdot \mathbf{n}_{s,i})^* - \tilde{\mathbf{F}}_e^\delta \cdot \mathbf{n}_{s,i})(\boldsymbol{\xi}_i^L) g'_L(\xi_{p_i}) dS_{\boldsymbol{\xi}} = \mathbf{0}. \end{aligned} \quad (1.36)$$

We now illustrate how to approximate $\tilde{\mathbf{F}}$ for various degrees. For $N = 1$, we need to approximate

$$\tilde{\mathbf{F}}^\delta = \tilde{\mathbf{f}}^\delta + \frac{\Delta t}{2} \partial_t \tilde{\mathbf{f}}^\delta,$$

so we need to approximate $\partial_t \tilde{\mathbf{f}}$, which we do as

$$\partial_t \tilde{\mathbf{f}} \approx \frac{\tilde{\mathbf{f}}^{n+1} - \tilde{\mathbf{f}}^{n-1}}{2 \Delta t} \approx \frac{\tilde{\mathbf{f}}(\mathbf{u} + \Delta t \mathbf{u}_t) - \tilde{\mathbf{f}}(\mathbf{u} - \Delta t \mathbf{u}_t)}{2 \Delta t} =: \partial_t \tilde{\mathbf{f}}^\delta. \quad (1.37)$$

We approximate \mathbf{u}_t as

$$\mathbf{u}_t = -\frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \tilde{\mathbf{f}}_e^\delta, \quad (1.38)$$

where $\tilde{\mathbf{f}}_e^\delta$ is the cell local approximation to the flux $\tilde{\mathbf{f}}_e^\delta$. For $N = 2$, we additionally need to approximate $\partial_{tt} \tilde{\mathbf{f}}$, which we do as

$$\begin{aligned} \partial_{tt} \tilde{\mathbf{f}} & \approx \frac{1}{\Delta t^2} (\tilde{\mathbf{f}}^{n+1} - 2 \tilde{\mathbf{f}}^n + \tilde{\mathbf{f}}^{n-1}) \\ & \approx \frac{1}{\Delta t^2} \left(\tilde{\mathbf{f}}\left(\mathbf{u} + \Delta t \mathbf{u}_t + \frac{\Delta t}{2} \mathbf{u}_{tt}\right) - 2 \tilde{\mathbf{f}}(\mathbf{u}) + \tilde{\mathbf{f}}\left(\mathbf{u} - \Delta t \mathbf{u}_t + \frac{\Delta t}{2} \mathbf{u}_{tt}\right) \right) \\ & =: \partial_{tt} \tilde{\mathbf{f}}^\delta, \end{aligned}$$

where we approximate \mathbf{u}_{tt} as

$$\mathbf{u}_{tt} = -\frac{1}{J} \nabla_{\boldsymbol{\xi}} \cdot \partial_t \tilde{\mathbf{f}}^\delta. \quad (1.39)$$

The procedure for other degrees shall be similar.

1.3.4. Free stream preservation for LWFR

We will show that the usual metric identities

$$\sum_{i=1}^3 \partial_{\xi_i} I^N(J \mathbf{a}^i) = \mathbf{0}$$

are sufficient for free stream preservation. To indicate that we are differentiation polynomial of degree N , we will use the operator $D_{\xi_i}^N$ and to indicate the derivatives used in computation of the metric terms, we will use operator D_{ξ_i} . We also define the gradient type operators as $D_{\boldsymbol{\xi}}^N = (D_{\xi_1}^N, D_{\xi_2}^N, D_{\xi_3}^N)$ and $D_{\boldsymbol{\xi}} = (D_{\xi_1}, D_{\xi_2}, D_{\xi_3})$. With these, the metric terms can be written as

$$J \mathbf{a}^i = (D_{\boldsymbol{\xi}} x_j) \times (D_{\boldsymbol{\xi}} x_k)$$

and the metric identities as

$$\sum_{i=1}^3 D_{\xi_i} I^N(J \mathbf{a}^i) = \mathbf{0}.$$

Update all following notations

If we assume $\mathbf{u}^n = \underline{\mathbf{c}}$, and $\mathbf{f}(\underline{\mathbf{c}}) = \underline{\mathbf{c}}$. We will begin by proving that

$$\tilde{\mathbf{F}}^\delta = \tilde{\mathbf{f}}^\delta.$$

In this case, $\tilde{\mathbf{f}}$ will be

$$\tilde{\mathbf{f}}_i = J \mathbf{a}^i \cdot \mathbf{c} = \sum_{n=1}^3 I^N(J a_n^i) \mathbf{c}_n.$$

This will give, using (1.38),

$$\begin{aligned} \mathbf{u}_t &= -\frac{1}{J} D_{\xi}^N \cdot \tilde{\mathbf{f}}_e^{\delta} = -\frac{1}{J} \sum_{i=1}^3 \partial_{\xi^i} \tilde{\mathbf{f}}_{e,i}^{\delta} \\ &= -\frac{1}{J} \sum_{i=1}^3 D_{\xi^i} \left(\sum_{n=1}^3 I^N(J a_n^i) \mathbf{c}_n \right) \\ &= -\sum_{n=1}^3 \left(\sum_{i=1}^3 D_{\xi^i} I^N(J a_n^i) \right) \mathbf{c}_n = 0, \end{aligned}$$

For $N=1$, by (1.37), this proves that

$$\partial_t \tilde{\mathbf{f}}^{\delta} = \frac{\tilde{\mathbf{f}}(\mathbf{u} + \Delta t \mathbf{u}_t) - \tilde{\mathbf{f}}(\mathbf{u} - \Delta t \mathbf{u}_t)}{2 \Delta t} = \mathbf{0}.$$

Thus, we obtain

$$\tilde{\mathbf{F}}^{\delta} = \tilde{\mathbf{f}}^{\delta} + \frac{\Delta t}{2} \partial_t \tilde{\mathbf{f}}^{\delta} = \tilde{\mathbf{f}}^{\delta}.$$

Building on this, for $N=2$, by (1.39),

$$\mathbf{u}_{tt} = -\frac{1}{J} \nabla_{\xi} \cdot \partial_t \tilde{\mathbf{f}}^{\delta} = \mathbf{0},$$

which will prove

$$\partial_{tt} \tilde{\mathbf{f}}^{\delta} = \mathbf{0},$$

and we get

$$\tilde{\mathbf{F}}^{\delta} = \tilde{\mathbf{f}}^{\delta} + \frac{\Delta t}{2} \partial_t \tilde{\mathbf{f}}^{\delta} + \frac{\Delta t^2}{3!} \partial_{tt} \tilde{\mathbf{f}}^{\delta} = \tilde{\mathbf{f}}^{\delta}.$$

The claim shall similarly hold for all degrees. Thus, substituting

$$\tilde{\mathbf{F}}^{\delta} = \tilde{\mathbf{f}}^{\delta} = \{J \mathbf{a}^i \cdot \mathbf{c}\}_{i=1}^3$$

in (1.36) gives

$$\begin{aligned} &\mathbf{u}^{n+1} - \mathbf{u}^n + \frac{1}{J} \Delta t \left(\sum_{i=1}^3 \partial_{\xi^i} (J \mathbf{a}^i) \right) \cdot \mathbf{c} \\ &+ \frac{1}{J} \Delta t \sum_{i=1}^3 \int_{\partial \Omega_{s,i}} ((J \mathbf{a}^i \cdot \mathbf{c})^* - J \mathbf{a}^i \cdot \mathbf{c}) (\xi_i^R) g_R'(\xi_{p_i}) dS_{\xi} \\ &+ \frac{1}{J} \Delta t \sum_{i=1}^3 \int_{\partial \Omega_{s,i}} ((J \mathbf{a}^i \cdot \mathbf{c})^* - J \mathbf{a}^i \cdot \mathbf{c}) (\xi_i^L) g_L'(\xi_{p_i}) dS_{\xi} = \mathbf{0}. \end{aligned} \tag{1.40}$$

The volume term vanishes by the metric identities and the surface terms vanish by conformality of the mesh.

1.3.5. Satisfying metric identities

Now that we have reduced metric identities to

$$\sum_{i=1}^3 \partial_{\xi^i} I^N(J \mathbf{a}^i) = \mathbf{0},$$

we show conditions under which they are satisfied.

LEMMA 1.5. $\nabla u \times \nabla v = -\nabla \times (v \nabla u) = \nabla \times (u \nabla v)$

Proof. We use the basic vector calculus identity

$$\nabla \times (v \nabla u) = \nabla v \times \nabla u + v \nabla \times \nabla u$$

We prove the identity as

$$\begin{aligned} \nabla \times (v \nabla u) &= (v (\nabla u))_{j,i} \epsilon_{ijk} \mathbf{e}_k \\ &= (v u_{,j})_{,i} \epsilon_{ijk} \mathbf{e}_k \\ &= v_{,i} u_{,j} \epsilon_{ijk} \mathbf{e}_k + v u_{,ij} \epsilon_{ijk} \mathbf{e}_k \\ &= \nabla v \times \nabla u + v \nabla \times \nabla u \end{aligned}$$

Since $\nabla \times \nabla u = 0$, we get the first identity. Swapping u and v , we get the second identity. \square

Using this lemma, we get

$$\nabla_\xi x_m \times \nabla_\xi x_l = -\nabla_\xi \times (x_l \nabla_\xi x_m).$$

Writing the left-hand side of this explicitly, we get

$$\begin{aligned} \nabla_\xi x_m \times \nabla_\xi x_l &= \left[\frac{\partial x_m}{\partial \eta} \frac{\partial x_l}{\partial \zeta} - \frac{\partial x_m}{\partial \zeta} \frac{\partial x_l}{\partial \eta} \right] \hat{x} + \left[\frac{\partial x_m}{\partial \zeta} \frac{\partial x_l}{\partial \xi} - \frac{\partial x_m}{\partial \xi} \frac{\partial x_l}{\partial \zeta} \right] \hat{y} \\ &\quad + \left[\frac{\partial x_m}{\partial \xi} \frac{\partial x_l}{\partial \eta} - \frac{\partial x_m}{\partial \eta} \frac{\partial x_l}{\partial \xi} \right] \hat{z}. \end{aligned} \quad (1.41)$$

Recall that

$$J \vec{a}^i = \vec{a}_j \times \vec{a}_k = \frac{\partial \vec{X}}{\partial \xi_j} \times \frac{\partial \vec{X}}{\partial \xi_k}$$

Using this, we are supposed to show

$$J a_n^i = J \vec{a}^i \cdot \hat{x}_n = -\hat{x}_i \cdot \nabla_\xi \times (x_l \nabla_\xi x_m), \quad i = 1, 2, 3, \quad n = 1, 2, 3, \quad (n, m, l) \text{ cyclic}.$$

We can see this, from $i = 1$

$$\begin{aligned} -\hat{x}_1 \cdot \nabla_\xi \times (x_l \nabla_\xi x_m) &= \frac{\partial x_m}{\partial \eta} \frac{\partial x_l}{\partial \zeta} - \frac{\partial x_m}{\partial \zeta} \frac{\partial x_l}{\partial \eta} \\ &= \frac{\partial x_m}{\partial \xi^2} \frac{\partial x_l}{\partial \xi^3} - \frac{\partial x_m}{\partial \xi^3} \frac{\partial x_l}{\partial \xi^2} \\ &= \frac{\partial \vec{X}}{\partial \xi_2} \times \frac{\partial \vec{X}}{\partial \xi_3} \cdot \hat{x}_n \end{aligned}$$

To see the general case, write

$$\begin{aligned} \nabla_\xi x_m \times \nabla_\xi x_l &= \sum_{i=1}^3 \left[\frac{\partial x_m}{\partial \xi^j} \frac{\partial x_l}{\partial \xi^k} - \frac{\partial x_m}{\partial \xi^k} \frac{\partial x_l}{\partial \xi^j} \right] \hat{x}_i \quad (i, j, k) \text{ cycle}, \\ &= \sum_{i=1}^3 \left(\frac{\partial \vec{X}}{\partial \xi_j} \times \frac{\partial \vec{X}}{\partial \xi_k} \cdot \hat{x}_n \right) \hat{x}_i \quad (n, m, l) \text{ cycle}. \end{aligned} \quad (1.42)$$

Thus, we get our claim

THEOREM 1.6.

$$J a_n^i = -\hat{x}_i \cdot \nabla_\xi \times (x_l \nabla_\xi x_m), \quad i = 1, 2, 3, \quad n = 1, 2, 3, \quad (n, m, l) \text{ cyclic}. \quad (1.43)$$

This is the curl form of metric terms. We make three observations with the curl form.

1. Notice that metric identities follow from these immediately since

$$\sum_{i=1}^3 \frac{\partial (J a_n^i)}{\partial \xi^i} = -\nabla_\xi \cdot (\nabla_\xi \times (x_l \nabla_\xi x_m)) = 0, \quad n = 1, 2, 3 \quad (n, m, l) \text{ cyclic}.$$

2. Also, the curl form is exactly the “conservative form” of $J\vec{a}^i$ introduced by Thomas and Lombard [18], who wrote the components explicitly:

$$\begin{aligned} J\vec{a}^1 &= \left[(y_\eta z)_\zeta - (y_\zeta z)_\eta \right] \hat{x} + \left[(z_\eta x)_\zeta - (z_\zeta x)_\eta \right] \hat{y} + \left[(x_\eta y)_\zeta - (x_\zeta y)_\eta \right] \hat{z}, \\ J\vec{a}^2 &= \left[(y_\zeta z)_\xi - (y_\xi z)_\zeta \right] \hat{x} + \left[(z_\zeta x)_\xi - (z_\xi x)_\zeta \right] \hat{y} + \left[(x_\zeta y)_\xi - (x_\xi y)_\zeta \right] \hat{z}, \\ J\vec{a}^3 &= \left[(y_\xi z)_\eta - (y_\eta z)_\xi \right] \hat{x} + \left[(z_\xi x)_\eta - (z_\eta x)_\xi \right] \hat{y} + \left[(x_\xi y)_\eta - (x_\eta y)_\xi \right] \hat{z}. \end{aligned}$$

3. This “conservative” form is not unique because from the lemma above

$$\nabla u \times \nabla v = -\nabla \times (v \nabla u) = \nabla \times (u \nabla v),$$

we could have also swapped x_m and x_l to write

$$Ja_n^i = -\hat{x}_i \cdot \nabla_\xi \times (x_m \nabla_\xi x_l), \quad i = 1, 2, 3, \quad n = 1, 2, 3, \quad (n, m, l) \text{ cyclic}.$$

Thus, we understand the “invariant form” of metric terms introduced in [19, 24], which using our notation, were written in [19, 24] as

$$J\vec{a}^i = \frac{1}{2} [(\vec{X}_{\xi^j} \times \vec{X})_{\xi^k} - (\vec{X}_{\xi^k} \times \vec{X})_{\xi^j}], \quad i = 1, 2, 3, \quad (i, j, k) \text{ cyclic}. \quad (1.44)$$

Simple manipulations show that it is the average of the two “conservative forms”, i.e.,

$$\begin{aligned} Ja_n^i &= -\frac{1}{2} \hat{x}_i \cdot \nabla_\xi \times [x_l \nabla_\xi x_m - x_m \nabla_\xi x_l], \quad i = 1, 2, 3, \\ n &= 1, 2, 3, \quad (n, m, l) \text{ cyclic}. \end{aligned}$$

Is that initial “-” not supposed to be there?

We are now ready to see three approaches for computing the metric terms

1. Cross product form

$$I^N(J\vec{a}^i) = I^N\left(\frac{\partial \mathbf{x}}{\partial \xi^j} \times \frac{\partial \mathbf{x}}{\partial \xi^k}\right), \quad i = 1, 2, 3, \quad (i, j, k) \text{ cyclic}. \quad (1.45)$$

Here, \mathbf{x} represents the mapping from the element to the reference element.

2. Conservative curl form

$$\begin{aligned} I^N(Ja_n^i) &= -\mathbf{e}_i \cdot \nabla_\xi \times (I^N(x_l \nabla_\xi x_m)), \\ i &= 1, 2, 3, \quad n = 1, 2, 3; (n, m, l) \text{ cyclic}. \end{aligned} \quad (1.46)$$

3. Invariant curl form

$$\begin{aligned} Ja_n^i &= -\frac{1}{2} \mathbf{e}_i \cdot \nabla_\xi \times [I^N(x_l \nabla_\xi x_m - x_m \nabla_\xi x_l)], \\ i &= 1, 2, 3 \quad n = 1, 2, 3, \quad (n, m, l) \text{ cyclic}. \end{aligned} \quad (1.47)$$

We will consider the evaluation of the metric terms in two and three space dimensions separately.

1.3.5.1. Evaluating metrics in two space dimensions

In two space dimensions, the cross-product form (1.45) of $J\vec{a}^i$ reduces to

$$\begin{aligned} J\vec{a}^1 &= \vec{a}^2 \times \vec{a}^3 = y_\eta \mathbf{e}_1 - x_\eta \mathbf{e}_2, \\ J\vec{a}^2 &= \vec{a}^3 \times \vec{a}^1 = -y_\xi \mathbf{e}_1 + x_\xi \mathbf{e}_2, \end{aligned} \quad (1.48)$$

where $\mathbf{x}(\xi, \eta) = x \mathbf{e}_1 + y \mathbf{e}_2$. In that case, we have the following result:

THEOREM 1.7. *On a well-constructed mesh in two space dimensions, the cross product form (1.45) of the metric terms satisfies the metric identity*

$$\vec{X} \in \mathbb{P}_N.$$

Proof. If $\vec{X} \in \mathbb{P}_N$, the 2D cross product form expression (1.48) gives us

$$J\vec{a}^i \in \mathbb{P}_N \quad i = 1, 2.$$

Thus,

$$I^N(Ja_n^i) = Ja_n^i.$$

Since the divergence of $J\vec{a}^i$ is zero, we get the metric identity.

On the other hand, if the element faces are not in \mathbb{P}_N (i.e., of degree greater than N), then

$$I^N(Ja_n^i) \neq Ja_n^i.$$

Since, in general, we can't commute differentiation and interpolation, we won't be able to obtain the zero divergence of $I^N(Ja_n^i)$. Thus, with the cross product form where mappings are not in \mathbb{P}_N , the metric identities are not satisfied. \square

Remark 1.8.

Remark 2. Theorem 3 says that the typical isoparametric approximation where the boundaries are approximated to the same order as the solution will satisfy the discrete metric identities and hence will be constant-state preserving. It also implies that using element boundary approximations that are lower order than the solution approximation order still gives a constant-state preserving approximation. This may be required, for example, when boundary surfaces are only known as low order splines or if the mesh generator can generate only low order elements. Finally, one might naively think that a more accurate representation of boundaries using higher order interpolants would be better. It is interesting to note that Theorem 3 says that approximating the boundaries to higher order does *not* help.

Remark 1.9. Finally, if we interpolate the mapping before differentiating, i.e., compute

$$\begin{aligned} I^N J\mathbf{a}^1 &= (I^N y)_\eta \mathbf{e}_1 - (I^N x)_\eta \mathbf{e}_2, \\ I^N J\mathbf{a}^2 &= -(I^N y)_\xi \mathbf{e}_1 + (I^N x)_\xi \mathbf{e}_2, \end{aligned}$$

then Theorem 1.7 holds and metric identities are satisfied.

[This is basically adding another interpolation to the mapping.](#)

This is analytically equivalent to computing the curl form in 2D as

$$\begin{aligned} I^N(Ja_n^i) &= -\mathbf{e}_i \cdot \nabla_\xi \times (I^N(x_l \nabla_\xi(I^N x_m))), \\ i &= 1, 2, \quad n = 1, 2, \quad (n, m, l) \text{ cyclic.} \end{aligned}$$

1.3.5.2. Evaluating metrics in three space dimensions

In 3D, the cross product form (1.45) **does not** satisfy the metric identities except in very special cases:

THEOREM 1.10. *We consider well-constructed mesh in three space dimensions with the cross product form (1.45). The metric identities are not satisfied if $q > N/2$. The metric identities are satisfied, however, if $q \leq N/2$.*

Proof. Unlike 2D, the cross products will now involve multiplication of degree N polynomials. So, the condition that $q \leq N/2$ is natural. \square

However, the other two forms - conservative curl form (1.46) and invariant curl form (1.47), always satisfy the metric identities, since the interpolation is performed before the curl is computed

THEOREM 1.11. *On a well-constructed mesh in three space dimensions, the conservative curl form (1.46) and invariant curl form (1.47) of the metric terms satisfy the metric identities for all mappings \mathbf{x} .*

Proof. If the conservative curl form is used, then

$$\sum_{i=1}^3 \frac{\partial I^N(Ja_n^i)}{\partial \xi^i} = -\nabla_\xi \cdot \nabla_\xi \times (I^N(x_l \nabla_\xi x_m)) = 0,$$

$$n = 1, 2, 3, \quad (n, m, l) \text{ cyclic},$$

so the result is established. Similarly, for the invariant curl form

$$\sum_{i=1}^3 \frac{\partial I^N(Ja_n^i)}{\partial \xi^i} = -\frac{1}{2} \nabla \cdot \nabla_\xi \times [I^N(x_l \nabla_\xi x_m - x_m \nabla_\xi x_l)] = 0, \quad \square$$

$$n = 1, 2, 3, \quad (n, m, l) \text{ cyclic}.$$

1.4. NON-CONSERVATIVE LAX-WENDROFF FLUX RECONSTRUCTION (FR) ON CURVILINEAR GRIDS

This scheme has been labeled non-conservative by [1] because the flux derivative on the scheme obtained after quadrature is not the flux derivative in (1.28), but the one in (6.39) of [2].

1.4.1. Non-conservative Discontinuous Galerkin (DG) method

We define degree N Lagrange polynomial basis $\{\ell_{ijk}\}$ on the reference cell $\Omega_s = [0, 1]^3$. Let \mathbf{u}^δ , \mathbf{f}^δ be the approximate solution and flux in the physical space, which need not be polynomials. Corresponding to each Ω_e , we define as reference map

$$\Theta_e: \Omega_s \rightarrow \Omega_e,$$

using which we can define degree N approximate solution and flux in the reference space

$$\hat{\mathbf{u}}_e^\delta(\boldsymbol{\xi}) = \sum_{i,j,k=1}^{N+1} \hat{u}_{e,ijk} \ell_{ijk}(\boldsymbol{\xi}),$$

$$\hat{\mathbf{f}}_e^\delta(\boldsymbol{\xi}) = \sum_{i,j,k=1}^{N+1} \mathbf{f}(\mathbf{u}_{ijk}) \ell_{ijk}(\boldsymbol{\xi}),$$

and the physical quantities are then defined implicitly

$$\mathbf{u}^\delta(\Theta_e^{-1}(\boldsymbol{\xi})) = \hat{\mathbf{u}}_e^\delta(\boldsymbol{\xi}),$$

$$\mathbf{f}^\delta(\Theta_e^{-1}(\boldsymbol{\xi})) = \hat{\mathbf{f}}_e^\delta(\boldsymbol{\xi}).$$

To obtain the non-conservative form, we take the DG scheme to be

$$\int \int_{\Omega_e} \left(\frac{\partial \hat{\mathbf{u}}_e^\delta}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{f}^\delta \right) \ell_{ijk}(\boldsymbol{\xi}) d\mathbf{x} + \int_{\partial\Omega_e} \mathbf{n} \cdot [\mathbf{f}^* - \mathbf{f}^\delta] \ell_{ij}(\boldsymbol{\xi}) ds = 0, \quad (1.49)$$

$$i, j, k = 1, \dots, N+1,$$

where $\ell_{ijk}(\boldsymbol{\xi})$ is a Lagrange polynomial polynomial in the reference element. We cannot compute a derivative in the physical variable, so the above $\nabla_{\mathbf{x}} \cdot \mathbf{f}^\delta$ actually refers to

$$\nabla_{\mathbf{x}} \cdot \mathbf{f}^\delta = (\nabla_{\mathbf{x}} \xi_i) \cdot (\partial_{\xi_i} \hat{\mathbf{f}}_e^\delta) = (\mathbf{a}_j \times \mathbf{a}_k) \cdot (\partial_{\xi_i} \hat{\mathbf{f}}_e^\delta),$$

where i, j, k form a cycle.

which is a quantity we can compute.

Thus, transforming to the reference coordinates, the DG scheme is

$$\int \int_{\Omega_s} \frac{\partial \hat{\mathbf{u}}_e^\delta}{\partial t} \ell_{p_1 p_2 p_3}(\boldsymbol{\xi}) J_e d\mathbf{x} + \int \int_{\Omega_s} \sum_{i=1}^3 J_e (\nabla_{\mathbf{x}} \xi_i) \cdot (\partial_{\xi_i} \hat{\mathbf{f}}_e^\delta) \ell_{p_1 p_2 p_3}(\boldsymbol{\xi}) d\mathbf{x} \quad (1.50)$$

$$+ \hat{\mathbf{b}}_{\text{DG}_e} = 0, \quad p_1, p_2, p_3 = 1, \dots, N+1,$$

where the boundary term $\hat{\mathbf{b}}_{\text{DG}_e}$ is given as

$$\hat{\mathbf{b}}_{\text{DG}_e} = \sum_{i=1}^3 \hat{\mathbf{b}}_{\text{DG}_e, i}^L + \hat{\mathbf{b}}_{\text{DG}_e, i}^R,$$

where i, L corresponds to the boundary face along i^{th} direction on face with 0 on i^{th} coordinate and i, R corresponds to boundary face along i^{th} direction on face with 1 on i^{th} coordinate.

$$\hat{\mathbf{b}}_{\text{DG}_e, i}^{L/R} = \int_{\partial\Omega_{s,i}^{L/R}} \mathbf{n}_i^{L/R} \cdot (\mathbf{f}_{e,i}^{*,L/R} - \mathbf{f}_{e,i}^{\delta,L/R}) \ell_{p_1 p_2 p_3} \bar{J}_{e,i}^{L/R} ds,$$

where

$$\mathbf{n}_i^{L/R} = \mathbf{a}_j \times \mathbf{a}_k / |\mathbf{a}_j \times \mathbf{a}_k|, \quad \bar{J}_{e,i}^{L/R} = |\mathbf{a}_j \times \mathbf{a}_k|,$$

where i, j, k form a cycle.

Thus, the boundary term is given by

$$\hat{\mathbf{b}}_{\text{DG}_e, i}^{L/R} = \int_{\partial\Omega_{s,i}^{L/R}} (\mathbf{a}_j \times \mathbf{a}_k) \cdot (\mathbf{f}_{e,i}^{*,L/R} - \mathbf{f}_{e,i}^{\delta,L/R}) \ell_{p_1 p_2 p_3} ds.$$

We choose the solution points to be Gauss-Legendre or Gauss-Lobatto points and the quadrature points to be the same. Now, we collocate the scheme at $\{\boldsymbol{\xi}_{p_1 p_2 p_3}\}_{p_i=1}^{N+1}$ and use the following notations for a fixed $\boldsymbol{\xi}_{pqr}$

$$\begin{aligned} \mathbf{w} &= w_{p_1} w_{p_2} w_{p_3}, & \mathbf{w}_i &= \mathbf{w} / w_{p_i}, \\ \ell &= \ell_{p_1 p_2 p_3}, & \ell_i(\boldsymbol{\xi}) &= \ell_{p_j}(\xi^j) \ell_{p_k}(\xi^k), \quad i, j, k \text{ are in a cycle.} \end{aligned}$$

Thus, the collocation scheme at a fixed $\boldsymbol{\xi}_{p_1 p_2 p_3}$ would be

$$\begin{aligned} \mathbf{w} \frac{d\hat{\mathbf{u}}_{p_1 p_2 p_3}}{dt} + \mathbf{w} \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot (\partial_{\xi_i} \hat{\mathbf{f}}_e^{\delta})(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ + \sum_{i=1}^3 \mathbf{w}_i (\mathbf{a}_j \times \mathbf{a}_k)_{i,L} \cdot (\mathbf{f}_{e,i}^{*,L} - \mathbf{f}_{e,i}^{\delta,L}) \ell_{p_i}(0) \ell_i(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ + \sum_{i=1}^3 \mathbf{w}_i (\mathbf{a}_j \times \mathbf{a}_k)_{i,R} \cdot (\mathbf{f}_{e,i}^{*,R} - \mathbf{f}_{e,i}^{\delta,R}) \ell_{p_i}(1) \ell_i(\boldsymbol{\xi}_{p_1 p_2 p_3}) = 0. \end{aligned}$$

where $\{w_p\}_{p=1}^{N+1}$ are the quadrature weights. Dividing by \mathbf{w} , we get

$$\begin{aligned} \frac{d\hat{\mathbf{u}}_{p_1 p_2 p_3}}{dt} + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot (\partial_{\xi_i} \hat{\mathbf{f}}_e^{\delta})(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k)_{i,L} \cdot (\mathbf{f}_{e,i}^{*,L} - \mathbf{f}_{e,i}^{\delta,L}) \frac{\ell_{p_i}(0)}{w_{p_i}} \ell_i(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k)_{i,R} \cdot (\mathbf{f}_{e,i}^{*,R} - \mathbf{f}_{e,i}^{\delta,R}) \frac{\ell_{p_i}(1)}{w_{p_i}} \ell_i(\boldsymbol{\xi}_{p_1 p_2 p_3}) = 0. \end{aligned}$$

It is known that

$$\frac{\ell_{p_i}(0)}{w_{p_i}}, \frac{\ell_{p_i}(1)}{w_{p_i}} = \begin{cases} g'_{\text{Radau},L}(\xi_{p_i}), g'_{\text{Radau},L}(\xi_{p_i}), & \text{Gauss-Legendre solution points and quadrature,} \\ g'_{\text{Hu},L}(\xi_{p_i}), g'_{\text{Hu},L}(\xi_{p_i}), & \text{Gauss-Lobatto solution points and quadrature.} \end{cases}$$

With $\frac{\ell_{p_i}(0)}{w_{p_i}}$, there must be a minus to obtain correction functions.

Thus, we obtain the scheme

$$\begin{aligned} \frac{d\hat{\mathbf{u}}_{e,p_1 p_2 p_3}}{dt} + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot (\partial_{\xi_i} \hat{\mathbf{f}}_e^{\delta})(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k)_{i,L} \cdot (\mathbf{f}_{e,i}^{*,L} - \mathbf{f}_{e,i}^{\delta,L}) g'_L(\xi_{p_i}) \ell_i(\boldsymbol{\xi}_{p_1 p_2 p_3}) \\ + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k)_{i,R} \cdot (\mathbf{f}_{e,i}^{*,R} - \mathbf{f}_{e,i}^{\delta,R}) g'_R(\xi_{p_i}) \ell_i(\boldsymbol{\xi}_{p_1 p_2 p_3}) = 0. \end{aligned} \tag{1.51}$$

1.4.2. Flux Reconstruction

We explain degree N Flux Reconstruction (FR) on a general curvilinear mesh defined in Section 1.1. We first introduce the interpolation operator I_N . For 1-D Lagrange polynomial basis $\{\ell_p(\xi)\}_{p=1}^{N+1}$ for solution points $\{\xi_p\}_{p=1}^{N+1}$ in $[-1, 1]$, we define the interpolation operator I^N for any \mathbf{u} to be

$$I^N(\mathbf{u})(\boldsymbol{\xi}) = \sum_{p,q,r=1}^{N+1} \mathbf{u}(\xi_p, \xi_q, \xi_r) \ell_p(\xi^1) \ell_q(\xi^2) \ell_r(\xi^3).$$

Corresponding to the element Ω_e , we define approximate polynomial and discontinuous flux polynomials to solve the transformed conservation law (1.28)

$$\begin{aligned} \tilde{\mathbf{u}}_e^\delta &= \tilde{\mathbf{u}}_e^\delta(\boldsymbol{\xi}, t) = J_e \mathbf{u}_e^\delta(\boldsymbol{\xi}, t), \\ \tilde{\mathbf{f}}_e^\delta &= \tilde{\mathbf{f}}_e^\delta(\boldsymbol{\xi}, t) = (\tilde{f}_{e,1}^\delta, \tilde{f}_{e,2}^\delta, \tilde{f}_{e,3}^\delta) \end{aligned}$$

where $\tilde{\mathbf{u}}_e^\delta$ is defined as

$$\tilde{\mathbf{u}}_e^\delta(\boldsymbol{\xi}, t) = \sum_{i,j,k=1}^{N+1} \tilde{\mathbf{u}}_{ijk} \ell_i(\xi^1) \ell_j(\xi^2) \ell_k(\xi^3),$$

and we solve for the unknowns $\tilde{\mathbf{u}}_{ijk}$, and

$$\mathbf{u}_{ijk} = J_e^{-1} \tilde{\mathbf{u}}_{ijk}.$$

The discontinuous flux on reference cell is defined as the polynomial

The discontinuous flux is defined to be the polynomial

$$\mathbf{f}_e^\delta(\boldsymbol{\xi}, t) = \sum_{i,j,k=1}^{N+1} \mathbf{f}(\mathbf{u}_{ijk}) \ell_i(\xi^1) \ell_j(\xi^2) \ell_k(\xi^3),$$

and the contravariant flux to be

$$\tilde{\mathbf{f}}_e^\delta = I^N(J \vec{\mathbf{a}}^i) \cdot \vec{\mathbf{F}}_e^\delta.$$

Remark 1.12. For the later derivation, we will not be treating $\tilde{\mathbf{f}}_e^\delta$ as a degree N polynomial, but as a degree $2N$ polynomial. Thus, we are not doing standard FR on the transformed conservation law (1.28). However, we choose to do it this way because it turns out to be the one equivalent to non-conservative form of DG, as defined by Cinchio.

The quantities in physical cell are defined implicitly as

$$\begin{aligned} \mathbf{u}^\delta(\mathbf{x}, t) &= J_e^{-1} \tilde{\mathbf{u}}_e^\delta(\Theta_e^{-1}(\boldsymbol{\xi}), t), \\ \mathbf{f}^\delta(\mathbf{x}, t) &= \mathbf{f}_e^\delta(\Theta_e^{-1}(\boldsymbol{\xi}), t). \end{aligned}$$

We shall usually suppress the subscript e indicating the physical element. With this, we get that FR scheme in reference cell given by

$$\frac{\partial \hat{u}^\delta}{\partial t} + \nabla_{\boldsymbol{\xi}} \cdot \hat{\mathbf{f}}^\delta + \hat{\mathbf{b}}_{\text{FR}_n} = 0, \quad (1.52)$$

where $\hat{\mathbf{b}}_{\text{FR}_n}$ is the correction term defined as

$$\hat{\mathbf{b}}_{\text{FR}_n}(\boldsymbol{\xi}) = \sum_{i=1}^3 g_L'(\xi_i) \Delta \hat{\mathbf{f}}_{i,L}^\delta + g_R'(\xi_i) \Delta \hat{\mathbf{f}}_{i,R}^\delta,$$

where i, L denotes the direction along ξ_i where the i^{th} coordinate is -1 and i, R is where i^{th} coordinate is $+1$, and

$$\Delta \hat{\mathbf{f}}_{i,L/R}^\delta = \hat{\mathbf{f}}_{i,L/R}^{*,\delta} - \hat{\mathbf{f}}_{i,L/R}^\delta.$$

Write this better. It is not direction, but location.

$$\Delta \hat{\mathbf{f}}_{i,L/R}^\delta = \Delta((\mathbf{a}_j \times \mathbf{a}_k) \cdot \mathbf{f}^\delta)_{i,L/R} = (\mathbf{a}_j \times \mathbf{a}_k)_{i,L/R} \cdot \Delta \mathbf{f}_{i,L/R}^\delta, \quad (1.53)$$

where we have used conformality of the mesh.

Remark 1.13. This is where we have used the fact that

$$\tilde{\mathbf{f}}_e^\delta = I^N(J\vec{a}^i) \cdot \vec{F}_e^\delta \neq I^N(I^N(J\vec{a}^i) \cdot I^N(\vec{F}_e^\delta)).$$

Using the metric identities

$$\begin{aligned} \nabla_{\xi} \cdot \hat{\mathbf{f}}^\delta &= \sum_{i=1}^3 \partial_{\xi_i} [(\mathbf{a}_j \times \mathbf{a}_k) \cdot \mathbf{f}^\delta] = \underbrace{\left[\sum_{i=1}^3 \partial_{\xi_i} (\mathbf{a}_j \times \mathbf{a}_k) \right]}_{=0} \cdot \mathbf{f}^\delta + \sum_{i=1}^3 [(\mathbf{a}_j \times \mathbf{a}_k) \cdot \partial_{\xi_i} \mathbf{f}^\delta] \\ &= \sum_{i=1}^3 [(\mathbf{a}_j \times \mathbf{a}_k) \cdot \partial_{\xi_i} \mathbf{f}^\delta] \\ &= \frac{\partial \hat{u}^\delta}{\partial t} + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot [\partial_{\xi_i} \mathbf{f}^\delta] \\ &\quad + \sum_{i=1}^3 [g'_L(\xi_i) (\mathbf{a}_j \times \mathbf{a}_k)_{i,L} \cdot \Delta \mathbf{f}_{i,L}^\delta + g'_R(\xi_i) (\mathbf{a}_j \times \mathbf{a}_k)_{i,R} \cdot \Delta \mathbf{f}_{i,R}^\delta] = 0 \end{aligned}$$

where, for $\mathbf{x} \in \Omega_e$,

$$\mathbf{f}^\delta(\mathbf{x}) = \mathbf{f}^\delta(\Theta_e(\xi)).$$

Since we would know the function as a polynomial mapping from $\xi \mapsto \mathbf{f}^\delta(\Theta_e^{-1}(\xi))$, we can easily differentiate it without needing the chain rule. This scheme is clearly equivalent to the collocated DG scheme (1.51).

It is clear that this is constant state preserving.

We will show that the non-conservative form of FR in previous section is equivalent to non-conservative form of DG, following the proof of [3]. To prove that, we multiply

1.4.3. Free stream preservation for Lax-Wendroff scheme

For a Lax-Wendroff, the update would be replaced by

$$\hat{\mathbf{u}}^{n+1} - \hat{\mathbf{u}}^n + \sum_{i=1}^3 (\mathbf{a}_j \times \mathbf{a}_k) \cdot [\partial_{\xi_i} \mathbf{F}^\delta + g'_L(\xi_i) \Delta \mathbf{F}_{i,L}^\delta + g'_R(\xi_i) \Delta \mathbf{F}_{i,R}^\delta] = 0,$$

where we have discretized the scheme in time and replaced the spatial quantities by polynomials.

Now, we assume $\mathbf{u} = \underline{\mathbf{c}}$, and $\mathbf{f}(\underline{\mathbf{c}}) = \mathbf{c}$. In the FR scheme, we only need to compute

$$\mathbf{F}^\delta = \sum_{m=0}^N \frac{\Delta t^m}{(m+1)!} \partial_t^m \mathbf{f}$$

Remark 1.14. It is because of the non-conservative form that we can work with temporal derivatives of \mathbf{f} instead of $\tilde{\mathbf{f}}$.

Let us illustrate this for $N = 1$, where we approximate

$$\partial_t \mathbf{f} \approx \frac{\mathbf{f}(\mathbf{u} + \mathbf{u}_t) + \mathbf{f}(\mathbf{u} - \mathbf{u}_t)}{2 \Delta t},$$

where we approximate

$$\begin{aligned} \mathbf{u}_t &\approx -\nabla_{\mathbf{x}} \cdot \mathbf{f} \\ &= 0, \end{aligned}$$

because we assumed that $\mathbf{f} = \mathbf{c}$. The same proof shall go forward for $N > 1$.

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