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Energy Stable Flux Reconstruction Schemes for Advection–Diffusion Problems on Tetrahedra

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Abstract The flux reconstruction (FR) methodology provides a unifying description of many high-order schemes, including a particular discontinuous Galerkin (DG) scheme and several spectral difference (SD) schemes. In addition, the FR methodology has been used to generate new classes of high-order schemes, including the recently discovered 'energy stable' FR schemes. These schemes, which are often referred to as VCJH (Vincent–Castonguay–Jameson–Huynh) schemes, are provably stable for linear advection–diffusion problems in 1D and on triangular elements. The VCJH schemes have been successfully applied to a wide variety of problems in 1D and 2D, ranging from linear advection–diffusion problems, to fluid mechanics problems requiring the solution of the compressible Navier–Stokes equations. Based on the results of these numerical experiments, it has been shown that certain VCJH schemes maintain the expected order of spatial accuracy and possess explicit time-step limits which rival those of the collocation-based nodal DG scheme. However, it remained to be seen whether the VCJH schemes could be extended to 3D on tetrahedral elements, enabling their convenient application to the complex geometries that arise in many real-world problems. For the first time, this article presents an extension of the VCJH schemes to tetrahedral elements. This work provides a formal proof of the stability of the new schemes and assesses their performance via numerical experiments on model problems.

Keywords High-order · Unstructured · Discontinuous Galerkin · Spectral difference · Flux reconstruction · Tetrahedra

Mathematics Subject Classification (2000) 65M12 · 65M60 · 65M70 · 35Q35 · 35L65 · 35Q30

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1 Introduction

It is generally believed that higher fidelity numerical methods are needed for solving many of the unsteady, compressible, viscous flow problems that arise in industrial settings. Currently, such problems are frequently solved using second-order methods on unstructured meshes of triangular and tetrahedral elements [20]. However, these second-order methods introduce numerical dissipation that interferes with the propagation of vortices and other time-dependent phenomena. As a result, there has been significant interest in developing high-order methods that are suitable for unstructured meshes (cf. the recent review article by Vincent and Jameson [34]). These high-order methods have the potential to produce less dissipation and to obtain more accurate results at lower computational cost [19]. However, these methods appear to be less robust and more difficult to implement than their low-order counterparts, and therefore, despite their promise, have yet to be adopted by the majority of fluid dynamicists.

In order to address this issue, there have been efforts to improve the flexibility and ease of implementation of high-order methods, and in particular the well-known discontinuous Galerkin (DG) methods. These efforts have brought about a rise in popularity of 'nodal' DG methods that omit the explicit use of quadratures (as described in [19]), allowing them to serve as simpler alternatives to the classical DG methods that utilize complex quadrature procedures (described in [3,4,11]). There have also been efforts to develop an alternative class of high-order methods referred to as spectral difference (SD) methods. The SD methods, originally proposed by Kopriva and Kolias [27] and generalized by Liu, Vinokur, and Wang [29], omit the explicit use of quadratures by employing a nodal representation of the solution, where the nodes are placed at the locations of the Chebyshev points. Finally, there have been efforts to develop the flux reconstruction (FR) methodology (discovered by Huynh [22]) which provides a unifying framework for a number of well-known nodal DG and SD schemes, and establishes an intuitive methodology for identifying new classes of robust high-order schemes. In particular, Huynh has used the FR methodology to identify new high-order schemes for advection and diffusion problems in 1D [22,23] and in 2D [23,24] on quadrilateral and triangular elements. In addition, Wang, Gao, Haga, and Yu have identified new schemes, referred to as correction procedure via reconstruction (CPR) schemes [18,39], which are a generalization of the FR schemes and the (closely related) lifting collocation penalty (LCP) schemes [15,17,35,36]. The CPR schemes have been successfully applied to a wide range of problems in 2D on quadrilateral and triangular elements [15,35,36] and in 3D on prismatic and tetrahedral elements [17,18]. The reader may consult [38] for a more comprehensive review of the CPR approach along with other FR (and FR-type) approaches.

As the discussion above indicates, there are many FR schemes to choose from. However, it is preferable to consider only those schemes whose stability can be rigorously established. Towards this end, Huynh has employed Fourier analysis [22,23], and Wang, Gao, Haga, and Yu have employed numerical experiments [15,17,18,35,36] in order to establish the stability of their respective classes of FR schemes. Alternatively, Jameson [25], Vincent et al. [33], Castonguay et al. [9,10], and Williams et al. [38] have employed an 'energy stability' approach to identify a particular class of stable FR schemes. This approach is more general than that of Fourier analysis and numerical experimentation, as it produces results which hold for all orders of accuracy on arbitrary unstructured grids. In [25], Jameson used this approach to identify a particular SD scheme that is provably stable for linear advection problems in 1D. Thereafter, Vincent et al. [33] extended this approach to identify an infinite range of 'energy stable' FR schemes that are provably stable for linear advection problems in 1D. These schemes, referred to as Vincent–Castonguay–Jameson–Huynh (VCJH) schemes, are parameterized by a single scalar c, and for an appropriate choice of this scalar, one can recover a collocation-based nodal DG scheme along with the SD scheme that Jameson identified in [25]. Most recently, Castonguay et al. [9,10] and Williams et al. [38] used the energy stability approach to identify a class of FR schemes that are provably stable for linear advection–diffusion problems in 1D and on triangular elements. These schemes (also referred to as VCJH schemes) are parameterized by two scalars c and κ, and for appropriate choices of these scalars, it can be shown that a collocation-based nodal DG scheme is recovered. In [38], the resulting schemes were successfully applied to linear and nonlinear advection–diffusion problems in 2D, and it was shown that certain VCJH schemes maintain the expected order of spatial accuracy while possessing explicit time-step limits that are more than 2x larger than those of the collocation-based nodal DG scheme.

To the authors' knowledge, a class of energy stable FR schemes has yet to be developed for advection–diffusion problems on tetrahedral elements. In this work, the FR approach that was proven to be stable for linear advection–diffusion problems on triangular elements in [9,10], and [38], will be extended to tetrahedral elements. This will result in a new class of high-order methods for unstructured meshes of tetrahedral elements.

The remainder of this article has the following structure. Section 2 describes the general FR approach for treating tetrahedral elements. Section 3 introduces the energy stable FR approach (i.e. the VCJH approach) for tetrahedral elements and proves the stability of this approach for linear advection–diffusion problems. Section 4 identifies values of the coefficients c and κ that preserve the spatial symmetry of the schemes. Section 5 proves that the resulting class of VCJH schemes is equivalent to a class of filtered DG schemes. Section 6 presents the VCJH schemes which have explicit time-step limits that are maximal (for linear advection problems). Finally, in an effort to further assess the capabilities of the VCJH schemes, section 7 presents the results of numerical experiments on a canonical linear advection–diffusion problem.

2 Flux Reconstruction for Advection–Diffusion Problems on Tetrahedral Elements

In what follows, the general FR methodology for advection–diffusion problems on triangular elements, described by Castonguay et al. [9,10] and Williams et al. [38], is extended to tetrahedral elements.

2.1 Preliminaries

Consider the 3D advection–diffusion equation which (in accordance with [5]) can be expressed as the following first-order system

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{f} = 0, \tag{1}$$

$$\mathbf{q} - \nabla u = 0, \tag{2}$$

where u is a scalar solution, t is time, ∇ is the gradient operator defined such that $\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$, $\mathbf{x} = (x, y, z) = (x_1, x_2, x_3)$ are spatial coordinates, $\mathbf{f} = \mathbf{f}(u, \mathbf{q})$ is an advective-diffusive flux, and $\mathbf{q}$ is an 'auxiliary variable.' One seeks a solution to the system given by Eqs. (1) and (2) within the 3D domain $\boldsymbol{\Omega}$ with boundary $\boldsymbol{\Gamma}$. Towards this end, the domain can be divided into N conforming, non-overlapping, straight-sided tetrahedral elements $\boldsymbol{\Omega}_k$ (where $k = 1, \ldots, N$), and within each element the solution u can be approximated by a function u_k^D which is continuously defined within $\boldsymbol{\Omega}_k$ and which vanishes outside

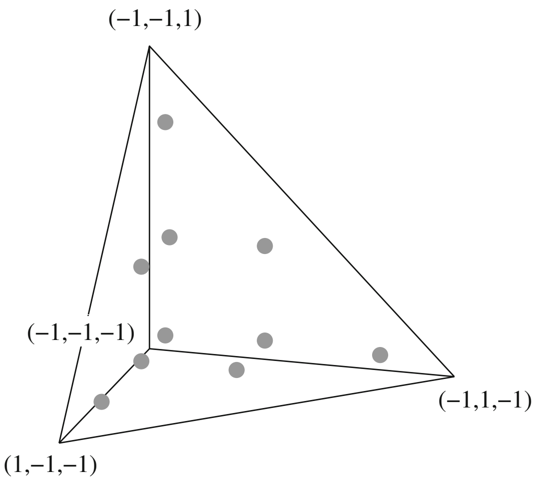


Fig. 1 Example of the $N_p = 10$ solution point locations (denoted by *spheres*) in the reference element for $p = 2$

of the element. The function u_k^D is labeled with a superscript D to indicate that, in general, it is discontinuous at the boundary between neighboring elements $\mathbf{\Omega}_k$ and $\mathbf{\Omega}_{k+1}$. In accordance with the traditional, discontinuous finite element approach (as described in [19]), u_k^D can be approximated using a polynomial of degree p that takes the following form

$$u_k^D = \sum_{i=1}^{N_p} (u_k^D)^i \, \ell_i \, (\mathbf{x}) \,, \tag{3}$$

where $(u_k^D)^i$ is the value of the solution at solution point i within $\mathbf{\Omega}_k$ and $\ell_i \, (\mathbf{x})$ is the multi-dimensional nodal basis function which assumes the value of 1 at solution point i and the value of 0 at all other solution points. Figure 1 shows an example of the $N_p = 10$ solution points which can be used to define a degree $p = 2$ polynomial approximation of the solution on the tetrahedron. In general, note that $N_p = \frac{(p+1)(p+2)(p+3)}{6}$ on the tetrahedron.

In a similar fashion, the auxiliary variable $\mathbf{q}$ and the flux $\mathbf{f}$ within $\mathbf{\Omega}_k$ can be approximated by vector-valued functions $\mathbf{q}_k^D$ and $\mathbf{f}_k^D$ (respectively) whose components are polynomials of degree p that are defined as follows

$$\mathbf{q}_k^D = \left(q_{x_k}^D, q_{y_k}^D, q_{z_k}^D\right) = \left(q_{1_k}^D, q_{2_k}^D, q_{3_k}^D\right),$$

$$\forall \, m = 1, 2, 3, \quad q_{m_k}^D = \sum_{i=1}^{N_p} (q_{m_k}^D)^i \, \ell_i \, (\mathbf{x}) \,, \tag{4}$$

$$\mathbf{f}_k^D = \left(f_{x_k}^D, f_{y_k}^D, f_{z_k}^D\right) = \left(f_{1_k}^D, f_{2_k}^D, f_{3_k}^D\right),$$

$$\forall \, m, \quad f_{m_k}^D = \sum_{i=1}^{N_p} (f_{m_k}^D)^i \, \ell_i \, (\mathbf{x}) \,, \tag{5}$$

where $(q_{m_k}^D)^i$ and $(f_{m_k}^D)^i$ are values of the m^{th} components of the auxiliary variable and the flux at solution point i. Note that, in general, the flux $(f_{m_k}^D)^i$ is a nonlinear function of both the solution $(u_k^D)^i$ and the auxiliary variable $(\mathbf{q}_k^D)^i$. Upon substituting u_k^D, $\mathbf{q}_k^D$, and $\mathbf{f}_k^D$ in place of u, $\mathbf{q}$, and $\mathbf{f}$ in Eqs. (1) and (2), one obtains

$$\frac{\partial u_k^D}{\partial t} + \nabla \cdot \mathbf{f}_k^D = 0, \tag{6}$$

$$\mathbf{q}_k^D - \nabla u_k^D = 0. \tag{7}$$

As currently constructed, Eqs. (6) and (7) involve only information that is local to the k^{th} element. However, in order to construct a valid numerical scheme, it is necessary to incorporate information from neighboring elements. Towards this end, the FR approach replaces the discontinuous flux $\mathbf{f}_k^D$ in Eq. (6) with a 'reconstructed flux' $\mathbf{f}_k$ of degree $p+1$ which is required to be continuous in the following sense: the normal components of $\mathbf{f}_k$ and $\mathbf{f}_{k+1}$ are required to be equivalent to one another on the boundary between neighboring elements $\boldsymbol{\Omega}_k$ and $\boldsymbol{\Omega}_{k+1}$. In addition, the FR approach replaces the discontinuous solution u_k^D in Eq. (7) with a reconstructed solution u_k of degree $p+1$ which is required to be continuous in the sense that u_k and u_{k+1} are required to be equivalent to one another on the boundary between $\boldsymbol{\Omega}_k$ and $\boldsymbol{\Omega}_{k+1}$. Upon replacing $\mathbf{f}_k^D$ and u_k^D with $\mathbf{f}_k$ and u_k in Eqs. (6) and (7), one obtains

$$\frac{\partial u_k^D}{\partial t} + \nabla \cdot \mathbf{f}_k = 0, \tag{8}$$

$$\mathbf{q}_k^D - \nabla u_k = 0. \tag{9}$$

Prior to solving Eqs. (8) and (9), it is convenient to first transform these equations *from* the domain of the physical element $\boldsymbol{\Omega}_k$ *to* the domain of a 'reference element' $\boldsymbol{\Omega}_S$. Towards this end, suppose that a mapping $\boldsymbol{\Theta}_k$ is defined between the physical coordinates $\mathbf{x}$ in $\boldsymbol{\Omega}_k$ and the reference coordinates $\hat{\mathbf{x}} = (\hat{x}, \hat{y}, \hat{z})$ in $\boldsymbol{\Omega}_S$. One may construct the Jacobian matrix $\mathbf{J}_k = \hat{\nabla}\boldsymbol{\Theta}_k$ (where $\hat{\nabla} = \left(\frac{\partial}{\partial \hat{x}}, \frac{\partial}{\partial \hat{y}}, \frac{\partial}{\partial \hat{z}}\right)$) and the Jacobian determinant $J_k = \det(\mathbf{J}_k)$. Next, one may use $\mathbf{J}_k$ and J_k in order to transform the physical quantities u_k, u_k^D, $\mathbf{f}_k$, and $\mathbf{q}_k^D$ defined on $\boldsymbol{\Omega}_k$ into reference quantities $\hat{u}$, $\hat{u}^D$, $\hat{\mathbf{f}}$, and $\hat{\mathbf{q}}^D$ defined on $\boldsymbol{\Omega}_S$ as follows

$$\hat{u} = J_k\, u_k\left(\boldsymbol{\Theta}_k\left(\hat{\mathbf{x}}\right), t\right), \qquad \hat{u}^D = J_k\, u_k^D\left(\boldsymbol{\Theta}_k\left(\hat{\mathbf{x}}\right), t\right), \tag{10}$$

$$\hat{\mathbf{f}} = J_k\, \mathbf{J}_k^{-1}\, \mathbf{f}_k, \qquad \hat{\mathbf{q}}^D = J_k\, \mathbf{J}_k^T\, \mathbf{q}_k^D = \hat{\nabla}\hat{u} = J_k\, \mathbf{J}_k^T\, \nabla u_k. \tag{11}$$

Note that, in conjunction with Eqs. (10) and (11), the following equations also hold

$$\nabla \cdot \mathbf{f}_k = J_k^{-1}\left(\hat{\nabla} \cdot \hat{\mathbf{f}}\right), \tag{12}$$

$$\nabla u_k \cdot \mathbf{f}_k = J_k^{-2}\left(\hat{\nabla}\hat{u} \cdot \hat{\mathbf{f}}\right), \tag{13}$$

$$\int_{\boldsymbol{\Omega}_k} u_k\left(\nabla \cdot \mathbf{f}_k\right)\, d\boldsymbol{\Omega}_k = J_k^{-1} \int_{\boldsymbol{\Omega}_S} \hat{u}\left(\hat{\nabla} \cdot \hat{\mathbf{f}}\right) d\boldsymbol{\Omega}_S, \tag{14}$$

$$\int_{\boldsymbol{\Omega}_k} \nabla u_k \cdot \mathbf{f}_k\, d\boldsymbol{\Omega}_k = J_k^{-1} \int_{\boldsymbol{\Omega}_S} \hat{\nabla}\hat{u} \cdot \hat{\mathbf{f}}\, d\boldsymbol{\Omega}_S, \tag{15}$$

$$\int_{\boldsymbol{\Gamma}_k} u_k\left(\mathbf{f}_k \cdot \mathbf{n}\right)\, d\boldsymbol{\Gamma}_k = J_k^{-1} \int_{\boldsymbol{\Gamma}_S} \hat{u}\left(\hat{\mathbf{f}} \cdot \hat{\mathbf{n}}\right) d\boldsymbol{\Gamma}_S. \tag{16}$$

In particular, Eq. (12) holds for general tetrahedral elements, and Eqs. (13)–(16) hold for straight-sided tetrahedral elements. The equations above (Eqs. (10)–(16)) will be used frequently in subsequent discussions. For now, consider substituting Eqs. (10)–(12) into Eqs. (8) and (9), in order to obtain the following

$$\frac{\partial \hat{u}^D}{\partial t} + \hat{\nabla} \cdot \hat{\mathbf{f}} = 0, \tag{17}$$

$$\hat{\mathbf{q}}^D - \hat{\nabla} \hat{u} = 0. \tag{18}$$

In what follows, the FR procedure for solving Eqs. (17) and (18) will be discussed.

2.2 The FR Procedure

The FR procedure for solving Eqs. (17) and (18) involves obtaining the unknown quantities $\hat{\mathbf{q}}^D$, the auxiliary variable in reference space, and $\frac{\partial \hat{u}^D}{\partial t}$, the time rate of change of the solution in reference space, from computations of (respectively) $\hat{\nabla}\hat{u}$, the gradient of the reconstructed solution in reference space, and $\hat{\nabla} \cdot \hat{\mathbf{f}}$, the divergence of the reconstructed flux in reference space.

2.2.1 Computing $\hat{\nabla}\hat{u}$, the Gradient of the Reconstructed Solution in Reference Space

In order to facilitate the computation of $\hat{\nabla}\hat{u}$, one must first formulate a more precise definition for $\hat{u}$. Towards this end, the FR approach requires $\hat{u}$ to take the following form on the element boundary $\mathbf{\Gamma}_S$

$$\hat{u}\Big|_{\mathbf{\Gamma}_S} = \hat{u}^{\star}\Big|_{\mathbf{\Gamma}_S} = \left(\hat{u}^D + \hat{u}^C\right)\Big|_{\mathbf{\Gamma}_S}, \tag{19}$$

where $\hat{u}^C$ is a 'solution correction' that corrects $\hat{u}^D$ in such a way that the sum of $\hat{u}^D$ and $\hat{u}^C$ assumes the value of $\hat{u}^{\star}$, the value of the common numerical solution in reference space. Equation (19) ensures that $\hat{u}$ (and thus u_k) is continuous at the boundary between neighboring elements $\mathbf{\Omega}_k$ and $\mathbf{\Omega}_{k+1}$. In practice, Eq. (19) is enforced pointwise at the $l = 1, \ldots, N_{fp}$ 'flux points' on the $f = 1, \ldots, N_{ef}$ faces of the element, as follows

$$\hat{u}_{f,l} = \hat{u}^{\star}_{f,l} = \hat{u}^D_{f,l} + \hat{u}^C_{f,l} \qquad \forall f, l \tag{20}$$

where (for example) $\hat{u}^D_{f,l}$ is the value of $\hat{u}^D$ at flux point l on face f.

For reference, the $f = 1, \ldots, 4$ faces of the tetrahedron are shown in Fig. 2, and the $l = 1, \ldots, 6$ flux points for the case of $f = 1$, $p = 2$ are shown in Fig. 3. Note that, in general $N_{fp} = (p+1)(p+2)/2$ and $N_{ef} = 4$ for a tetrahedron.

Now, having formulated $\hat{u}$ in terms of $\hat{u}^D$ and $\hat{u}^C$ via Eqs. (19) and (20), one may formulate $\hat{\nabla}\hat{u}$ in a similar fashion as follows

$$\hat{\nabla}\hat{u} = \hat{\nabla}\hat{u}^D + \hat{\nabla}\hat{u}^C, \tag{21}$$

where $\hat{\nabla}\hat{u}^D$ can be computed by applying the gradient operator $\hat{\nabla}$ to $\hat{u}^D$, and $\hat{\nabla}\hat{u}^C$ can be computed by applying the 'lifting operators' (or 'correction fields') $\psi_{f,l}$ to values of $\hat{u}^C_{f,l}$ as follows

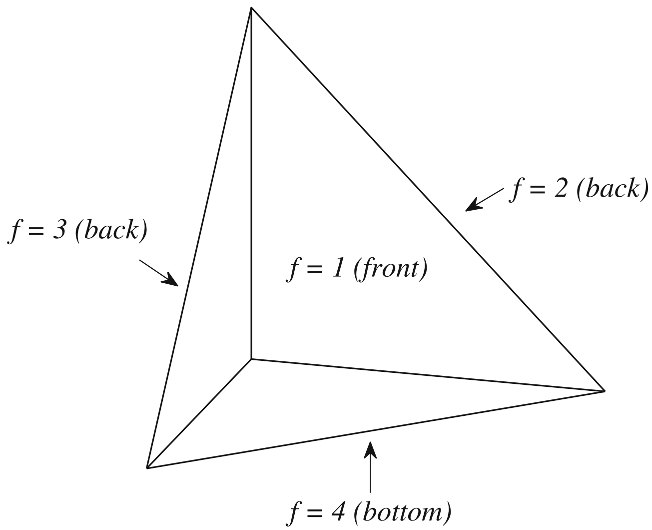
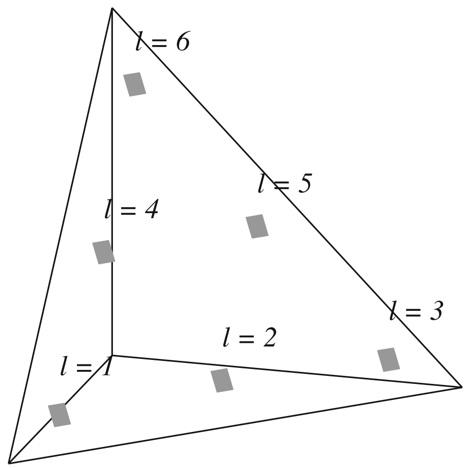


Fig. 2 Example of the numbering convention for the faces on the reference element

Fig. 3 Example of the numbering convention for the flux points on the reference element for $p = 2$. The flux points (denoted by *squares*) are shown for the face $f = 1$



$$\hat{\nabla}\hat{u}^C\left(\hat{\mathbf{x}}\right) = \sum_{f=1}^{N_{fe}}\sum_{l=1}^{N_{fp}} \hat{u}^C_{f,l}\hat{\mathbf{n}}_{f,l}\ \psi_{f,l}\left(\hat{\mathbf{x}}\right)$$
$$= \sum_{f=1}^{N_{fe}}\sum_{l=1}^{N_{fp}} \left[\hat{u}^{\star}_{f,l} - \hat{u}^D_{f,l}\right]\hat{\mathbf{n}}_{f,l}\ \psi_{f,l}\left(\hat{\mathbf{x}}\right). \tag{22}$$

The lifting operators $\psi_{f,l}(\hat{\mathbf{x}})$ are designed to 'lift' (or transform) values of $\hat{u}^C$ defined on $\mathbf{\Gamma}_S$ into values of $\hat{\nabla}\hat{u}^C$ defined on $\mathbf{\Omega}_S$. In order to ensure that the operators perform this task, they are defined such that $\psi_{f,l} \equiv \hat{\nabla}\cdot\mathbf{g}_{f,l}$, where each $\mathbf{g}_{f,l}$ is a vector-valued 'correction function' associated with flux point l on face f. In addition, the normal component of each correction function ($\mathbf{g}_{f,l}\cdot\hat{\mathbf{n}}$) is required to satisfy the following condition

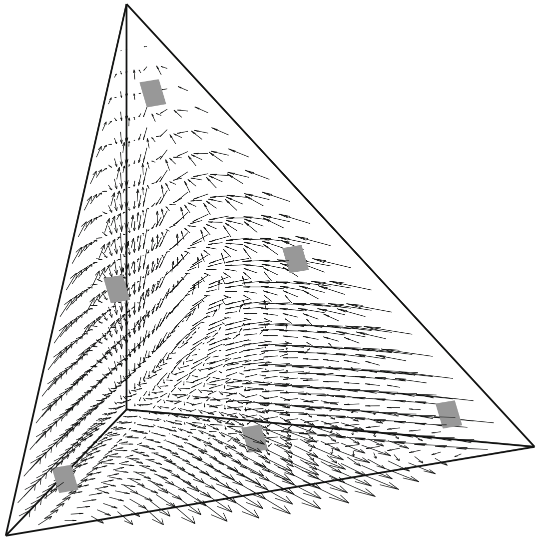


Fig. 4 Example of a vector correction function $\mathbf{g}_{f,l}$ associated with flux point $f = 1, l = 2$ for $p = 2$

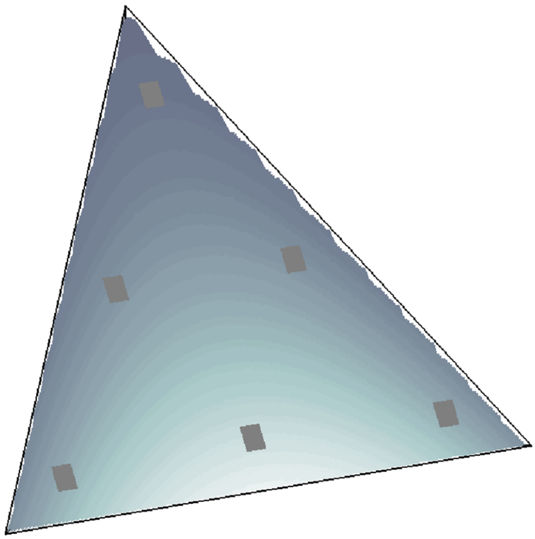


Fig. 5 Contours of a correction field $\psi_{f,l}$ (where $\psi_{f,l} \equiv \hat{\nabla} \cdot \mathbf{g}_{f,l}$) associated with flux point $f = 1, l = 2$ for $p = 2$

$$\mathbf{g}_{f,l}\left(\hat{\mathbf{x}}_{v,w}\right) \cdot \hat{\mathbf{n}}_{v,w} = \begin{cases} 1 & \text{if } v = f \text{ and } w = l \\ 0 & \text{if } v \neq f \text{ or } w \neq l \end{cases} \quad . \tag{23}$$

Furthermore, $\mathbf{g}_{f,l}\left(\hat{\mathbf{x}}\right)$ is required to belong to the Raviart–Thomas space of degree p (defined in [31]) in order to ensure that the following holds

$$\psi_{f,l} \equiv \hat{\nabla} \cdot \mathbf{g}_{f,l} \in P_p\left(\boldsymbol{\Omega}_S\right), \qquad \mathbf{g}_{f,l} \cdot \hat{\mathbf{n}} \in R_p\left(\boldsymbol{\Gamma}_S\right), \tag{24}$$

where $P_p\left(\boldsymbol{\Omega}_S\right)$ and $R_p\left(\boldsymbol{\Gamma}_S\right)$ are spaces which contain the polynomials of degree $\leq p$ on $\boldsymbol{\Omega}_S$ and $\boldsymbol{\Gamma}_S$, respectively. In [38], Williams et al. showed that Eqs. (23) and (24) ensure that $\psi_{f,l}$ serves as a lifting operator that transforms $\hat{u}^C$ defined on $\boldsymbol{\Gamma}_S$ into $\hat{\nabla}\hat{u}^C$ defined on $\boldsymbol{\Omega}_S$.

Figures 4 and 5 show an example of a vector correction function $\mathbf{g}_{f,l}$ and an associated correction field (lifting operator) $\psi_{f,l}$, for the case of $p = 2$.

2.2.2 Computing $\hat{\nabla} \cdot \hat{\mathbf{f}}$, the Divergence of the Reconstructed Flux in Reference Space

One must now define a precise form for $\hat{\mathbf{f}}$ in order to facilitate the computation of $\hat{\nabla} \cdot \hat{\mathbf{f}}$. Towards this end, the normal component of $\hat{\mathbf{f}}$ is required to satisfy the following equation

$$\hat{\mathbf{f}} \cdot \hat{\mathbf{n}}\Big|_{\boldsymbol{\Gamma}_S} = \hat{\mathbf{f}}^{\star} \cdot \hat{\mathbf{n}}\Big|_{\boldsymbol{\Gamma}_S} = \left(\hat{\mathbf{f}}^D + \hat{\mathbf{f}}^C\right) \cdot \hat{\mathbf{n}}\Big|_{\boldsymbol{\Gamma}_S}, \tag{25}$$

where $\hat{\mathbf{f}}^D = \hat{\mathbf{f}}^D\left(\hat{u}^D, \hat{\mathbf{q}}^D\right)$ is the discontinuous flux ($\mathbf{f}_k^D = \mathbf{f}_k^D\left(u_k^D, \mathbf{q}_k^D\right)$) in reference space, and where $\hat{\mathbf{f}}^C$ is a 'corrective flux' which corrects $\hat{\mathbf{f}}^D$ in such a way that the sum of the normal components of $\hat{\mathbf{f}}^D$ and $\hat{\mathbf{f}}^C$ equals the normal component of $\hat{\mathbf{f}}^{\star}$, the common numerical flux in reference space. Equation (25) ensures that the normal component of $\hat{\mathbf{f}}$ (and thus $\mathbf{f}_k$) is continuous at the boundary between neighboring elements. In practice, Eq. (25) is enforced pointwise as follows

$$\hat{\mathbf{f}}_{f,l} \cdot \hat{\mathbf{n}}_{f,l} = \hat{\mathbf{f}}^{\star}_{f,l} \cdot \hat{\mathbf{n}}_{f,l} = \left(\hat{\mathbf{f}}^D_{f,l} + \hat{\mathbf{f}}^C_{f,l}\right) \cdot \hat{\mathbf{n}}_{f,l} \qquad \forall f, l. \tag{26}$$

Now, having obtained a definition of $\hat{\mathbf{f}}$ in terms of $\hat{\mathbf{f}}^D$ and $\hat{\mathbf{f}}^C$, one can obtain a similar definition of $\hat{\nabla} \cdot \hat{\mathbf{f}}$ as follows

$$\hat{\nabla} \cdot \hat{\mathbf{f}} = \hat{\nabla} \cdot \hat{\mathbf{f}}^D + \hat{\nabla} \cdot \hat{\mathbf{f}}^C, \tag{27}$$

where $\hat{\nabla} \cdot \hat{\mathbf{f}}^D$ is obtained by applying the divergence operator $\hat{\nabla} \cdot$ to $\hat{\mathbf{f}}^D$, and $\hat{\nabla} \cdot \hat{\mathbf{f}}^C$ is obtained by applying lifting operators (correction fields) $\phi_{f,l}$ to values of $\hat{\mathbf{f}}^C_{f,l}$, as follows

$$\begin{aligned} \hat{\nabla} \cdot \hat{\mathbf{f}}^C &= \sum_{f=1}^{N_{fe}} \sum_{l=1}^{N_{fp}} \left[\hat{\mathbf{f}}^C_{f,l} \cdot \hat{\mathbf{n}}_{f,l}\right] \phi_{f,l} \\ &= \sum_{f=1}^{N_{fe}} \sum_{l=1}^{N_{fp}} \left[\left(\hat{\mathbf{f}}^{\star}_{f,l} - \hat{\mathbf{f}}^D_{f,l}\right) \cdot \hat{\mathbf{n}}_{f,l}\right] \phi_{f,l}. \end{aligned} \tag{28}$$

In Eq. (28), each correction field $\phi_{f,l}$ is defined as the divergence of a vector correction function $\mathbf{h}_{f,l}$. The functions $\mathbf{h}_{f,l}$ are required to possess the same properties as the functions $\mathbf{g}_{f,l}$ (which were defined previously). This ensures that the resulting FR schemes are conservative as shown by Castonguay et al. [10].

2.2.3 Obtaining a Final System of Equations

Upon substituting the expressions for $\hat{\nabla} \cdot \hat{\mathbf{f}}$ (Eqs. (27) and (28)) and $\hat{\nabla}\hat{u}$ (Eqs. (21) and (22)) into Eqs. (17) and (18), respectively, one obtains a complete description of the FR approach on the reference element $\boldsymbol{\Omega}_S$, as follows

$$\begin{aligned} &\frac{\partial \hat{u}^D}{\partial t} + \hat{\nabla} \cdot \hat{\mathbf{f}}^D + \hat{\nabla} \cdot \hat{\mathbf{f}}^C \\ &\quad = \frac{\partial \hat{u}^D}{\partial t} + \hat{\nabla} \cdot \hat{\mathbf{f}}^D + \sum_{f=1}^{N_{fe}} \sum_{l=1}^{N_{fp}} \left[\left(\hat{\mathbf{f}}^{\star}_{f,l} - \hat{\mathbf{f}}^D_{f,l}\right) \cdot \hat{\mathbf{n}}_{f,l}\right] \phi_{f,l} = 0, \end{aligned} \tag{29}$$

$$\hat{\mathbf{q}}^D - \hat{\nabla}\hat{u}^D - \hat{\nabla}\hat{u}^C$$
$$= \hat{\mathbf{q}}^D - \hat{\nabla}\hat{u}^D - \sum_{f=1}^{N_{fe}}\sum_{l=1}^{N_{fp}}\left[\hat{u}^{\star}_{f,l} - \hat{u}^D_{f,l}\right]\hat{\mathbf{n}}_{f,l}\ \psi_{f,l} = 0. \tag{30}$$

Equations (29) and (30) can be evaluated at the N_p solution points within $\mathbf{\Omega}_S$ in order to yield $4N_p$ equations for the $4N_p$ unknowns $(\frac{\partial \hat{u}^D}{\partial t})^1, \ldots, (\frac{\partial \hat{u}^D}{\partial t})^{Np}$ and $(\hat{\mathbf{q}}^D)^1, \ldots, (\hat{\mathbf{q}}^D)^{Np}$.

The behavior of the FR scheme defined by Eqs. (29) and (30) is determined by six factors:

1. The locations of the solution points $\hat{\mathbf{x}}_i$ within the element.
2. The locations of the flux points $\hat{\mathbf{x}}_{f,l}$ on the boundary of the element.
3. The procedure for computing the common numerical solution values $\hat{u}^{\star}_{f,l}$.
4. The procedure for computing the common numerical flux values $\hat{\mathbf{f}}^{\star}_{f,l}$.
5. The procedure for computing the solution correction fields $\psi_{f,l}$.
6. The procedure for computing the flux correction fields $\phi_{f,l}$.

If appropriate procedures are chosen for computing the common numerical solution values $\hat{u}^{\star}_{f,l}$, the common numerical flux values $\hat{\mathbf{f}}^{\star}_{f,l}$, the solution correction fields $\psi_{f,l}$, and the flux correction fields $\phi_{f,l}$, the FR schemes can be proven stable for linear advection–diffusion problems, independent of the locations of the solution points $\hat{\mathbf{x}}_i$ and flux points $\hat{\mathbf{x}}_{f,l}$. This will be shown in the following section.

3 Proof of Stability of VCJH Schemes for Linear Advection–Diffusion Problems

In this section, it will be shown that if the solution and flux correction fields $\psi_{f,l}$ and $\phi_{f,l}$ are chosen to be the 'VCJH correction fields', and if the common numerical solution values $\hat{u}^{\star}_{f,l}$ and common numerical flux values $\hat{\mathbf{f}}^{\star}_{f,l}$ are chosen appropriately, the ensuing FR schemes are stable for linear advection–diffusion problems.

3.1 Preliminaries

In order to examine the stability of the FR approach, it is useful to reformulate the approach on the physical element $\mathbf{\Omega}_k$. On $\mathbf{\Omega}_k$, Eqs. (29) and (30) of the FR approach can be expressed succinctly as follows

$$\frac{\partial u^D_k}{\partial t} + \nabla \cdot \mathbf{f}^D_k + \nabla \cdot \mathbf{f}^C_k = 0, \tag{31}$$
$$\mathbf{q}^D_k - \nabla u^D_k - \nabla u^C_k = 0, \tag{32}$$

where the reference quantities (defined on $\mathbf{\Omega}_S$) in Eqs. (29) and (30) were converted into physical quantities (defined on $\mathbf{\Omega}_k$) in Eqs. (31) and (32) via the transformations in Eqs. (10)–(12).

The FR approach for solving Eqs. (31) and (32) is considered to be 'energy stable' if

$$\sum_{k=1}^{N}\left(\frac{\mathrm{d}}{\mathrm{d}t}\|u^D_k\|^2\right) \le 0, \tag{33}$$

or equivalently

$$\sum_{k=1}^{N}\left(\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}\right)\le 0, \tag{34}$$

where $\mathbf{U}_k=\left[(u_k^D)^1\ \ldots (u_k^D)^{N_p}\right]^T$ is a vector containing the solution values,

$$\|\mathbf{U}_k\|_{\widetilde{\mathbf{M}}}=\mathbf{U}_k^T\,\widetilde{\mathbf{M}}^k\,\mathbf{U}_k \tag{35}$$

is a matrix-based norm, and $\widetilde{\mathbf{M}}^k$ is a symmetric positive-definite matrix. Note that the precise definition of $\widetilde{\mathbf{M}}^k$ will be given later on in this section.

In Eq. (34), the squared norm of the solution $\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}$ characterizes the energy of the solution. Therefore, Eq. (34) is a condition that ensures 'energy stability', because it insists that the time rate of change of the solution energy is non-positive.

It will be shown that Eq. (34) holds for a particular class of FR schemes, referred to as the VCJH schemes. The proof of stability of the VCJH schemes will consist of lemmas and a final theorem proving the stability of the schemes. In particular, the lemmas will summarize intermediate results which will be obtained from manipulating Eqs. (31) and (32), and the theorem will combine these results in order to prove that Eq. (34) holds.

Lemma 3.1 *Given that Eq. (31) holds for all FR schemes and provided that the flux correction functions and fields ($\mathbf{h}_{f,l}$ and $\phi_{f,l}$) are chosen to be the VCJH correction functions and fields, the following result holds*

$$\int\limits_{\boldsymbol{\Omega}_k}\frac{\partial u_k^D}{\partial t}\ell_j\,d\boldsymbol{\Omega}_k+\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v}c_{vw}\int\limits_{\boldsymbol{\Omega}_k}\frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\,d\boldsymbol{\Omega}_k$$
$$+\int\limits_{\boldsymbol{\Omega}_k}\left(\nabla\cdot\mathbf{f}_k^D\right)\ell_j\,d\boldsymbol{\Omega}_k=-\int\limits_{\boldsymbol{\Gamma}_k}\left(\mathbf{f}_k^C\cdot\mathbf{n}\right)\ell_j\,d\boldsymbol{\Gamma}_k, \tag{36}$$

where V_S is the volume of the reference element $\boldsymbol{\Omega}_S$, each c_{vw} is a constant which parameterizes $\phi_{f,l}$ (and thus $\mathbf{h}_{f,l}$), and each $\hat{D}^{(p,v,w)}$ is a derivative operator which will be subsequently defined.

Proof Consider defining a derivative operator $\hat{D}^{(p,v,w)}$ of degree p as follows

$$\hat{D}^{(p,v,w)}(\cdot)=\frac{\partial^p(\cdot)}{\partial\hat{x}^{(p-v+1)}\partial\hat{y}^{(v-w)}\partial\hat{z}^{(w-1)}}, \tag{37}$$

where $v=1,\ldots,p$ and $w=1,\ldots,v$. Note that, upon substituting all possible combinations of v and w into Eq. (37), one recovers the $(p+1)(p+2)/2$ distinct derivatives of degree p that exist in 3D.

One may apply $\hat{D}^{(p,v,w)}$ to Eq. (31) as follows

$$\frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)+\hat{D}^{(p,v,w)}\left(\nabla\cdot\mathbf{f}_k^D\right)+\hat{D}^{(p,v,w)}\left(\nabla\cdot\mathbf{f}_k^C\right)$$
$$=\frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)+\hat{D}^{(p,v,w)}\left(\nabla\cdot\mathbf{f}_k^C\right)=0, \tag{38}$$

where terms involving derivatives of the physical quantities w.r.t. the reference coordinates (i.e. terms such as $\hat{D}^{(p,v,w)}\left(u_k^D\right)$) are computed via the chain rule, and where $\hat{D}^{(p,v,w)}\left(\nabla\cdot\mathbf{f}_k^D\right)=0$ because $\nabla\cdot\mathbf{f}_k^D$ is a degree $p-1$ polynomial.

On multiplying Eq. (38) by $\hat{D}^{(p,v,w)}\left(\ell_j\right)$ and integrating over $\mathbf{\Omega}_k$, one obtains the following

$$\int_{\mathbf{\Omega}_k} \frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\mathbf{\Omega}_k + \int_{\mathbf{\Omega}_k} \hat{D}^{(p,v,w)}\left(\nabla\cdot\mathbf{f}_k^C\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\mathbf{\Omega}_k = 0. \tag{39}$$

Upon substituting Eq. (12) (with $\mathbf{f}^C$ in place of $\mathbf{f}$) into Eq. (39) and defining $\hat{\ell}_j \equiv J_k\,\ell_j$, one obtains

$$\begin{aligned}&\int_{\mathbf{\Omega}_k} \frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\mathbf{\Omega}_k \\ &\quad + \frac{1}{J_k}\int_{\mathbf{\Omega}_k} \hat{D}^{(p,v,w)}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right)\, d\mathbf{\Omega}_S = 0.\end{aligned} \tag{40}$$

On noting that $\hat{D}^{(p,v,w)}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)$ and $\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right)$ are constants because $\hat{\nabla}\cdot\hat{\mathbf{f}}^C$ and $\hat{\ell}_j$ are degree p polynomials, one obtains

$$\int_{\mathbf{\Omega}_k} \frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\mathbf{\Omega}_k + \frac{V_S}{J_k}\hat{D}^{(p,v,w)}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right) = 0. \tag{41}$$

Consider multiplying Eq. (41) by constant coefficients c_{vw}, and thereafter summing over v and w as follows

$$\begin{aligned}&\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\int_{\mathbf{\Omega}_k} \frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\mathbf{\Omega}_k \\ &\quad + \frac{V_S}{J_k}\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\hat{D}^{(p,v,w)}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right) = 0.\end{aligned} \tag{42}$$

The double summation in Eq. (42) contains $(p+1)(p+2)/2$ terms, one for each of the distinct $(p+1)(p+2)/2$ derivative operators of degree p that can be formed in 3D. As a result, the term of the form $\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\hat{D}^{(p,v,w)}(\cdot)$ is a general, weighted sum of all distinct derivatives of degree p.

Next, it should be noted that if $\hat{\mathbf{f}}^C$ and $\hat{\nabla}\cdot\hat{\mathbf{f}}^C$ are constructed using the VCJH correction functions $\mathbf{h}_{f,l}$ (which were discussed in section 2.2.2) and the VCJH fields $\phi_{f,l}$ (which have yet to be precisely defined), the following identity holds

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\,\hat{D}^{(p,v,w)}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right) = \int_{\mathbf{\Gamma}_S}\left(\hat{\mathbf{f}}^C\cdot\hat{\mathbf{n}}\right)\hat{\ell}_j\, d\mathbf{\Gamma}_S - \int_{\mathbf{\Omega}_S}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)\hat{\ell}_j\, d\mathbf{\Omega}_S. \tag{43}$$

For details on how the fields $\phi_{f,l}$ are constructed so as to ensure that Eq. (43) holds, please consult "Appendix A".

Upon substituting Eq. (43) into Eq. (42) and rearranging the result, one obtains

$$\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\int_{\boldsymbol{\Omega}_k}\frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\boldsymbol{\Omega}_k$$
$$+\frac{1}{J_k}\left[\int_{\boldsymbol{\Gamma}_S}\left(\hat{\mathbf{f}}^C\cdot\hat{\mathbf{n}}\right)\hat{\ell}_j\, d\boldsymbol{\Gamma}_S-\int_{\boldsymbol{\Omega}_S}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^C\right)\hat{\ell}_j\, d\boldsymbol{\Omega}_S\right]=0. \tag{44}$$

On substituting Eqs. (14) and (16) with $\hat{\mathbf{f}}^C$, $\mathbf{f}_k^C$, $\hat{\ell}_j$, and ℓ_j in place of $\hat{\mathbf{f}}$, $\mathbf{f}_k$, $\hat{u}$, and u_k into Eq. (44), one obtains

$$\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\int_{\boldsymbol{\Omega}_k}\frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\, d\boldsymbol{\Omega}_k$$
$$+\int_{\boldsymbol{\Gamma}_k}\left(\mathbf{f}_k^C\cdot\mathbf{n}\right)\ell_j\, d\boldsymbol{\Gamma}_k-\int_{\boldsymbol{\Omega}_k}\left(\nabla\cdot\mathbf{f}_k^C\right)\ell_j\, d\boldsymbol{\Omega}_k=0. \tag{45}$$

Setting Eq. (45) aside for the moment, consider multiplying Eq. (31) by the test function ℓ_j and integrating over $\boldsymbol{\Omega}_k$, as follows

$$\int_{\boldsymbol{\Omega}_k}\frac{\partial u_k^D}{\partial t}\ell_j\, d\boldsymbol{\Omega}_k+\int_{\boldsymbol{\Omega}_k}\left(\nabla\cdot\mathbf{f}_k^D\right)\ell_j\, d\boldsymbol{\Omega}_k+\int_{\boldsymbol{\Omega}_k}\left(\nabla\cdot\mathbf{f}_k^C\right)\ell_j\, d\boldsymbol{\Omega}_k=0. \tag{46}$$

Upon summing Eqs. (46) and (45), and rearranging the result, one obtains Eq. (36). This completes the proof of Lemma 3.1. □

Lemma 3.2 *Given that Eq. (32) holds for all FR schemes and provided that the solution correction functions and fields ($\mathbf{g}_{f,l}$ and $\psi_{f,l}$) are chosen to be the VCJH correction functions and fields, the following result holds*

$$\int_{\boldsymbol{\Omega}_k}\mathbf{q}_k^D\cdot\mathcal{L}_{m,j}\, d\boldsymbol{\Omega}_k+\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v}\kappa_{vw}\int_{\boldsymbol{\Omega}_k}\hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\boldsymbol{\Omega}_k$$
$$-\int_{\boldsymbol{\Omega}_k}\nabla u_k^D\cdot\mathcal{L}_{m,j}\, d\boldsymbol{\Omega}_k=\int_{\boldsymbol{\Gamma}_k}u_k^C\left(\mathcal{L}_{m,j}\cdot\mathbf{n}\right)d\boldsymbol{\Gamma}_k, \tag{47}$$

where each κ_{vw} is a constant which parameterizes $\psi_{f,l}$ (and thus $\mathbf{g}_{f,l}$), and each $\mathcal{L}_{m,j}$ is a vectorial generalization of the nodal basis function ℓ_j, i.e. $\mathcal{L}_{1,j}=\mathcal{L}_{x,j}\equiv\left(\ell_j,0,0\right)$, $\mathcal{L}_{2,j}=\mathcal{L}_{y,j}\equiv\left(0,\ell_j,0\right)$, and $\mathcal{L}_{3,j}=\mathcal{L}_{z,j}\equiv\left(0,0,\ell_j\right)$.

Proof Consider applying the derivative operator $\hat{D}^{(p,v,w)}$ to both sides of Eq. (32) as follows

$$\hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)-\hat{D}^{(p,v,w)}\left(\nabla u_k^D\right)-\hat{D}^{(p,v,w)}\left(\nabla u_k^C\right)$$
$$=\hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)-\hat{D}^{(p,v,w)}\left(\nabla u_k^C\right)=0, \tag{48}$$

where $\hat{D}^{(p,v,w)}\left(\nabla u_k^D\right)=0$ because ∇u_k^D is a degree $p-1$ polynomial.

Upon taking the dot product of Eq. (48) with $\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)$ and integrating over $\boldsymbol{\Omega}_k$, one obtains

$$\int\limits_{\boldsymbol{\Omega}_k} \hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\boldsymbol{\Omega}_k - \int\limits_{\boldsymbol{\Omega}_k} \hat{D}^{(p,v,w)}\left(\nabla u_k^C\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\boldsymbol{\Omega}_k = 0. \tag{49}$$

Next, one may define $\hat{\mathcal{L}}_{\hat{m},j} \equiv J_k\,\mathbf{J}_k^{-1}\mathcal{L}_{m,j}$ (where $\hat{m} = \hat{1}, \hat{2}, \hat{3}$, $\hat{\mathcal{L}}_{\hat{1},j} = \hat{\mathcal{L}}_{\hat{x},j}$, $\hat{\mathcal{L}}_{\hat{2},j} = \hat{\mathcal{L}}_{\hat{y},j}$, and $\hat{\mathcal{L}}_{\hat{3},j} = \hat{\mathcal{L}}_{\hat{z},j}$), and derive the following identity from Eq. (11), with u_k^C, $\mathcal{L}_{m,j}$, $\hat{u}^C$, and $\hat{\mathcal{L}}_{\hat{m},j}$ in place of u_k, $\mathbf{f}_k$, $\hat{u}$, and $\hat{\mathbf{f}}$,

$$\hat{D}^{(p,v,w)}\left(\nabla u_k^C\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right) = \left(J_k^{-2}\right)\hat{D}^{(p,v,w)}\left(\hat{\nabla}\hat{u}^C\right)\cdot\hat{D}^{(p,v,w)}\left(\hat{\mathcal{L}}_{\hat{m},j}\right). \tag{50}$$

On substituting Eq. (50) into Eq. (49), one obtains

$$\int\limits_{\boldsymbol{\Omega}_k} \hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\boldsymbol{\Omega}_k - \frac{1}{J_k}\int\limits_{\boldsymbol{\Omega}_S} \hat{D}^{(p,v,w)}\left(\hat{\nabla}\hat{u}^C\right)\cdot\hat{D}^{(p,v,w)}\left(\hat{\mathcal{L}}_{\hat{m},j}\right)d\boldsymbol{\Omega}_S = 0. \tag{51}$$

Upon multiplying Eq. (51) by constant coefficients κ_{vw}, summing over v and w, and noting that $\hat{D}^{(p,v,w)}\left(\hat{\nabla}\hat{u}^C\right)$ and $\hat{D}^{(p,v,w)}\left(\hat{\mathcal{L}}_{\hat{m},j}\right)$ are constant vectors because the components of $\hat{\nabla}\hat{u}^C$ and $\hat{\mathcal{L}}_{\hat{m},j}$ are degree p polynomials, one obtains the following

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v}\kappa_{vw}\int\limits_{\boldsymbol{\Omega}_k} \hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\boldsymbol{\Omega}_k - \frac{V_S}{J_k}\sum_{v=1}^{p+1}\sum_{w=1}^{v}\kappa_{vw}\,\hat{D}^{(p,v,w)}\left(\hat{\nabla}\hat{u}^C\right)\cdot\hat{D}^{(p,v,w)}\left(\hat{\mathcal{L}}_{\hat{m},j}\right) = 0. \tag{52}$$

Next, it should be noted that if $\hat{\nabla}\hat{u}^C$ is constructed using VCJH correction fields $\psi_{f,l}$ (where $\psi_{f,l} = \hat{\nabla}\cdot\mathbf{g}_{f,l}$ and each $\mathbf{g}_{f,l}$ is a VCJH correction function as discussed in section 2.2.1), the following identity holds

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v}\kappa_{vw}\,\hat{D}^{(p,v,w)}\left(\hat{\nabla}\hat{u}^C\right)\cdot\hat{D}^{(p,v,w)}\left(\hat{\mathcal{L}}_{\hat{m},j}\right) = \int\limits_{\boldsymbol{\Gamma}_S}\hat{u}^C\left(\hat{\mathcal{L}}_{\hat{m},j}\cdot\hat{\mathbf{n}}\right)d\boldsymbol{\Gamma}_S - \int\limits_{\boldsymbol{\Omega}_S}\hat{\nabla}\hat{u}^C\cdot\hat{\mathcal{L}}_{\hat{m},j}\,d\boldsymbol{\Omega}_S. \tag{53}$$

On substituting Eq. (53) into Eq. (52) and manipulating the result, one obtains

$$\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v}\kappa_{vw}\int\limits_{\boldsymbol{\Omega}_k} \hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\boldsymbol{\Omega}_k - \frac{1}{J_k}\left[\int\limits_{\boldsymbol{\Gamma}_S}\hat{u}^C\left(\hat{\mathcal{L}}_{\hat{m},j}\cdot\hat{\mathbf{n}}\right)d\boldsymbol{\Gamma}_S - \int\limits_{\boldsymbol{\Omega}_S}\hat{\nabla}\hat{u}^C\cdot\hat{\mathcal{L}}_{\hat{m},j}\,d\boldsymbol{\Omega}_S\right] = 0. \tag{54}$$

Upon substituting Eqs. (15) and (16) with u_k^C, $\mathcal{L}_{m,j}$, $\hat{u}^C$, and $\hat{\mathcal{L}}_{\hat{m},j}$ in place of u_k, $\mathbf{f}_k$, $\hat{u}$, and $\hat{\mathbf{f}}$ into Eq. (54), one obtains

$$\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v}\kappa_{vw}\int\limits_{\mathbf{\Omega}_k}\hat{D}^{(p,v,w)}\left(\mathbf{q}_k^D\right)\cdot\hat{D}^{(p,v,w)}\left(\mathcal{L}_{m,j}\right)d\mathbf{\Omega}_k$$
$$-\int\limits_{\mathbf{\Gamma}_k}u_k^C\left(\mathcal{L}_{m,j}\cdot\mathbf{n}\right)d\mathbf{\Gamma}_k+\int\limits_{\mathbf{\Omega}_k}\nabla u_k^C\cdot\mathcal{L}_{m,j}\,d\mathbf{\Omega}_k=0. \tag{55}$$

Setting this equation aside for the moment, consider taking the dot product of Eq. (32) with $\mathcal{L}_{m,j}$ and integrating over $\mathbf{\Omega}_k$, in order to obtain

$$\int\limits_{\mathbf{\Omega}_k}\mathbf{q}_k^D\cdot\mathcal{L}_{m,j}\,d\mathbf{\Omega}_k-\int\limits_{\mathbf{\Omega}_k}\nabla u_k^D\cdot\mathcal{L}_{m,j}\,d\mathbf{\Omega}_k-\int\limits_{\mathbf{\Omega}_k}\nabla u_k^C\cdot\mathcal{L}_{m,j}\,d\mathbf{\Omega}_k=0. \tag{56}$$

On summing Eqs. (56) and (55) and manipulating the result, one obtains Eq. (47). This completes the proof of Lemma 3.2. □

Lemma 3.3 *Suppose that the VCJH schemes (for which Lemmas 3.1 and 3.2 hold) are employed to solve the linear advection–diffusion equation for which the flux* $\mathbf{f}$ *takes the following form*

$$\mathbf{f}=\mathbf{f}_{adv}+\mathbf{f}_{dif}=(\mathbf{a}\,u)-(b\,\mathbf{q}), \tag{57}$$

where $\mathbf{a}$ *is a constant vector of wave speeds* $\mathbf{a}=(a_x,a_y,a_z)=(a_1,a_2,a_3)$ *and* $b\geq 0$ *is a constant coefficient of diffusivity. Then the following reformulation of the VCJH schemes (in terms of matrices) holds*

$$\widetilde{\mathbf{M}}^k\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k+\mathbf{S}^k\mathbf{A}\mathbf{U}_k-b\,\mathbf{S}^k\mathbf{Q}_k=\int\limits_{\mathbf{\Gamma}_k}\left[\left(\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)-(\mathbf{a}\,u-b\,\mathbf{q})^\star\right)\cdot\mathbf{n}\right]\mathbf{L}\,d\mathbf{\Gamma}_k, \tag{58}$$

$$\widetilde{\mathcal{M}}^k\,\mathbf{Q}_k-\mathcal{S}^k\mathbf{U}_k=-\int\limits_{\mathbf{\Gamma}_k}\left(u_k^D-u^\star\right)\mathbf{N}\mathbf{L}\,d\mathbf{\Gamma}_k, \tag{59}$$

where $\mathbf{U}_k$ *is a vector of solution values,* $\mathbf{Q}_k$ *is a vector of auxiliary variable values,* $\widetilde{\mathbf{M}}^k$ *and* $\widetilde{\mathcal{M}}^k$ *are positive-definite mass matrices (provided that* $c_{vw}\geq 0$ *and* $\kappa_{vw}\geq 0$*),* $\mathbf{S}^k$ *and* $\mathcal{S}^k$ *are stiffness matrices,* $\mathbf{A}$ *is a matrix of wave speeds,* $\mathbf{N}$ *is a matrix of face normals, and* $\mathbf{L}$ *is a vector of nodal basis functions. Note that these matrix and vector quantities will be defined more precisely in what follows. Note also that a relatively simple, analogous matrix formulation was constructed for the case of 1D advection by Allaneau and Jameson in* [1].

Proof Upon substituting expressions for the discontinuous flux $\mathbf{f}_k^D=\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)$ and the flux correction $\mathbf{f}_k^C=\mathbf{f}^\star-\mathbf{f}_k^D=(\mathbf{a}\,u-b\,\mathbf{q})^\star-\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)$ into Eq. (36), and insisting that the result holds for all j, one obtains

$$\forall j\quad\int\limits_{\mathbf{\Omega}_k}\frac{\partial u_k^D}{\partial t}\ell_j\,d\mathbf{\Omega}_k+\frac{1}{V_S}\sum_{v=1}^{p+1}\sum_{w=1}^{v}c_{vw}\int\limits_{\mathbf{\Omega}_k}\frac{\partial}{\partial t}\left(\hat{D}^{(p,v,w)}\left(u_k^D\right)\right)\hat{D}^{(p,v,w)}\left(\ell_j\right)\,d\mathbf{\Omega}_k$$
$$+\int\limits_{\mathbf{\Omega}_k}\nabla\cdot\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)\ell_j\,d\mathbf{\Omega}_k=\int\limits_{\mathbf{\Gamma}_k}\left(\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)-(\mathbf{a}\,u-b\,\mathbf{q})^\star\right)\cdot\mathbf{n}\,\ell_j\,d\mathbf{\Gamma}_k. \tag{60}$$

Also, on substituting an expression for the solution correction $u_k^C = \left(u^\star - u_k^D\right)$ into Eq. (47), and insisting that the result hold for all j and m, one obtains

$$\forall j, m \int_{\boldsymbol{\Omega}_k} \mathbf{q}_k^D \cdot \mathcal{L}_{m,j}\, d\boldsymbol{\Omega}_k + \frac{1}{V_S} \sum_{v=1}^{p+1} \sum_{w=1}^{v} \kappa_{vw} \int_{\boldsymbol{\Omega}_k} \hat{D}^{(p,v,w)} \left(\mathbf{q}_k^D\right) \cdot \hat{D}^{(p,v,w)} \left(\mathcal{L}_{m,j}\right) d\boldsymbol{\Omega}_k$$
$$- \int_{\boldsymbol{\Omega}_k} \nabla u_k^D \cdot \mathcal{L}_{m,j}\, d\boldsymbol{\Omega}_k = - \int_{\boldsymbol{\Gamma}_k} \left(u_k^D - u^\star\right) \mathbf{n} \cdot \mathcal{L}_{m,j}\, d\boldsymbol{\Gamma}_k. \tag{61}$$

Equations (60) and (61) can be manipulated and recast into matrix form. Towards this end, consider modifying Eq. (60) by transforming the second integral on the left hand side (LHS) from an integral over $\boldsymbol{\Omega}_k$ into an integral over $\boldsymbol{\Omega}_S$, as follows

$$\forall j \int_{\boldsymbol{\Omega}_k} \frac{\partial u_k^D}{\partial t} \ell_j\, d\boldsymbol{\Omega}_k + \frac{J_k}{V_S} \sum_{v=1}^{p+1} \sum_{w=1}^{v} c_{vw} \int_{\boldsymbol{\Omega}_S} \frac{\partial}{\partial t} \left(\hat{D}^{(p,v,w)} \left(u_k^D \left(\hat{\mathbf{x}}\right)\right)\right) \hat{D}^{(p,v,w)} \left(\ell_j \left(\hat{\mathbf{x}}\right)\right)\, d\boldsymbol{\Omega}_S$$
$$+ \int_{\boldsymbol{\Omega}_k} \nabla \cdot \left(\mathbf{a}\, u_k^D - b\, \mathbf{q}_k^D\right) \ell_j\, d\boldsymbol{\Omega}_k = \int_{\boldsymbol{\Gamma}_k} \left(\left(\mathbf{a}\, u_k^D - b\, \mathbf{q}_k^D\right) - \left(\mathbf{a}\, u - b\, \mathbf{q}\right)^\star\right) \cdot \mathbf{n}\, \ell_j\, d\boldsymbol{\Gamma}_k, \tag{62}$$

where the quantities $u_k^D\left(\hat{\mathbf{x}}\right)$ and $\ell_j\left(\hat{\mathbf{x}}\right)$ are defined via the mapping $\boldsymbol{\Theta}_k\left(\hat{\mathbf{x}}\right)$ as follows

$$u_k^D \left(\hat{\mathbf{x}}\right) \equiv u_k^D \left(\boldsymbol{\Theta}_k \left(\hat{\mathbf{x}}\right)\right) = u_k^D \left(\mathbf{x}\right) \equiv u_k^D, \tag{63}$$
$$\ell_j \left(\hat{\mathbf{x}}\right) \equiv \ell_j \left(\boldsymbol{\Theta}_k \left(\hat{\mathbf{x}}\right)\right) = \ell_j \left(\mathbf{x}\right) \equiv \ell_j. \tag{64}$$

Upon applying the same procedure to the second integral on the LHS of Eq. (61), one obtains

$$\forall j, m \int_{\boldsymbol{\Omega}_k} \mathbf{q}_k^D \cdot \mathcal{L}_{m,j}\, d\boldsymbol{\Omega}_k + \frac{J_k}{V_S} \sum_{v=1}^{p+1} \sum_{w=1}^{v} \kappa_{vw} \int_{\boldsymbol{\Omega}_S} \hat{D}^{(p,v,w)} \left(\mathbf{q}_k^D \left(\hat{\mathbf{x}}\right)\right) \cdot \hat{D}^{(p,v,w)} \left(\mathcal{L}_{m,j} \left(\hat{\mathbf{x}}\right)\right) d\boldsymbol{\Omega}_S$$
$$- \int_{\boldsymbol{\Omega}_k} \nabla u_k^D \cdot \mathcal{L}_{m,j}\, d\boldsymbol{\Omega}_k = - \int_{\boldsymbol{\Gamma}_k} \left(u_k^D - u^\star\right) \mathbf{n} \cdot \mathcal{L}_{m,j}\, d\boldsymbol{\Gamma}_k, \tag{65}$$

where

$$\mathbf{q}_k^D \left(\hat{\mathbf{x}}\right) \equiv \mathbf{q}_k^D \left(\boldsymbol{\Theta}_k \left(\hat{\mathbf{x}}\right)\right) = \mathbf{q}_k^D \left(\mathbf{x}\right) \equiv \mathbf{q}_k^D, \tag{66}$$
$$\mathcal{L}_{m,j} \left(\hat{\mathbf{x}}\right) \equiv \mathcal{L}_{m,j} \left(\boldsymbol{\Theta}_k \left(\hat{\mathbf{x}}\right)\right) = \mathcal{L}_{m,j} \left(\mathbf{x}\right) \equiv \mathcal{L}_{m,j}. \tag{67}$$

Now, Eqs. (62) and (65) can be recast in matrix form as follows

$$\left(\mathbf{M}^k + \frac{J_k}{N_p} \sum_{v=1}^{p+1} \sum_{w=1}^{v} c_{vw} \left(\hat{\mathbf{D}}^{(p,v,w)}\right)^T \hat{\mathbf{D}}^{(p,v,w)}\right) \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{U}_k + \sum_{m=1}^{3} \left(a_m \mathbf{S}_m^k \mathbf{U}_k - b\, \mathbf{S}_m^k \mathbf{Q}_{m_k}\right)$$
$$= \int_{\boldsymbol{\Gamma}_k} \left[\left(\left(\mathbf{a}\, u_k^D - b\, \mathbf{q}_k^D\right) - \left(\mathbf{a}\, u - b\, \mathbf{q}\right)^\star\right) \cdot \mathbf{n}\right] \mathbf{L}\, d\boldsymbol{\Gamma}_k, \tag{68}$$

$$\forall m, \quad \left(\mathbf{M}^k + \frac{J_k}{N_p} \sum_{v=1}^{p+1} \sum_{w=1}^{v} \kappa_{vw} \left(\hat{\mathbf{D}}^{(p,v,w)} \right)^T \hat{\mathbf{D}}^{(p,v,w)} \right) \mathbf{Q}_{m_k} - \mathbf{S}_m^k \mathbf{U}_k$$
$$= - \int_{\boldsymbol{\Gamma}_k} \left(u_k^D - u^\star \right) n_m \, \mathbf{L} \, d\boldsymbol{\Gamma}_k, \tag{69}$$

where $\mathbf{M}^k \in \mathbb{R}^{N_p \times N_p}$ is the local mass matrix with entries

$$\left[\mathbf{M}^k \right]_{ij} = \int_{\boldsymbol{\Omega}_k} \ell_i \left(\mathbf{x} \right) \ell_j \left(\mathbf{x} \right) \, d\boldsymbol{\Omega}_k = \int_{\boldsymbol{\Omega}_k} \ell_i \, \ell_j \, d\boldsymbol{\Omega}_k, \tag{70}$$

$\mathbf{S}_m^k \in \mathbb{R}^{N_p \times N_p}$ is the local stiffness matrix with entries

$$\left[\mathbf{S}_m^k \right]_{ij} = \int_{\boldsymbol{\Omega}_k} \ell_i \left(\mathbf{x} \right) \frac{\partial \ell_j \left(\mathbf{x} \right)}{\partial x_m} \, d\boldsymbol{\Omega}_k = \int_{\boldsymbol{\Omega}_k} \ell_i \frac{\partial \ell_j}{\partial x_m} \, d\boldsymbol{\Omega}_k, \tag{71}$$

$\hat{\mathbf{D}}^{(p,v,w)}$ is the matrix form of the derivative operator $\hat{D}^{(p,v,w)}$ defined such that

$$\left[\hat{\mathbf{D}}^{(p,v,w)} \, \mathbf{U}_k \right]_i \equiv \hat{D}^{(p,v,w)} \left(u_k^D \left(\hat{\mathbf{x}} \right) \right) \Big|_{\hat{\mathbf{x}}_i} = \left[\sum_{J=1}^{N_p} \left(u_k^D \right)_J \hat{D}^{(p,v,w)} \left(\ell_J \left(\hat{\mathbf{x}} \right) \right) \right]_{\hat{\mathbf{x}}_i}, \tag{72}$$

$\mathbf{U}_k = \left[(u_k^D)^1 \ldots (u_k^D)^{N_p} \right]^T$ is a vector containing the solution values, $\mathbf{Q}_{m_k} = \left[(q_{m_k}^D)^1 \ldots (q_{m_k}^D)^{N_p} \right]^T$ are vectors containing the auxiliary variable values, and $\mathbf{L} = \mathbf{L}\left(\mathbf{x}\right) = \left[\ell_1 \left(\mathbf{x} \right) \ldots \ell_{N_p} \left(\mathbf{x} \right) \right]^T$ is a vector containing the nodal basis functions.

Equations (68) and (69) can be simplified by introducing the following block matrix definitions (in terms of cartesian coordinates x, y, and z)

$$\mathcal{M}^k = \begin{bmatrix} \mathbf{M}^k & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}^k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{M}^k \end{bmatrix}, \tag{73}$$

$$\mathbf{S}^k = \left[\mathbf{S}_x^k \;\; \mathbf{S}_y^k \;\; \mathbf{S}_z^k \right], \qquad \mathcal{S}^k = \begin{bmatrix} \mathbf{S}_x^k \\ \mathbf{S}_y^k \\ \mathbf{S}_z^k \end{bmatrix}, \tag{74}$$

$$\mathbf{Q}_k = \begin{bmatrix} \mathbf{Q}_{x_k} \\ \mathbf{Q}_{y_k} \\ \mathbf{Q}_{z_k} \end{bmatrix}, \qquad \mathbf{A} = \begin{bmatrix} a_x \mathbf{I} \\ a_y \mathbf{I} \\ a_z \mathbf{I} \end{bmatrix}, \qquad \mathbf{N} = \begin{bmatrix} n_x \mathbf{I} \\ n_y \mathbf{I} \\ n_z \mathbf{I} \end{bmatrix}, \tag{75}$$

where $\mathbf{I} \in \mathbb{R}^{N_p \times N_p}$. In addition, one may define the following matrices in order to further simply the notation

$$\mathbf{K}^k = \frac{J_k}{N_p} \sum_{v=1}^{p+1} \sum_{w=1}^{v} c_{vw} \left(\hat{\mathbf{D}}^{(p,v,w)} \right)^T \hat{\mathbf{D}}^{(p,v,w)}, \tag{76}$$

$$\mathcal{K}^k = \frac{J_k}{N_p} \sum_{v=1}^{p+1} \sum_{w=1}^{v} \kappa_{vw} \begin{bmatrix} \left(\hat{\mathbf{D}}^{(p,v,w)}\right)^T \hat{\mathbf{D}}^{(p,v,w)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(\hat{\mathbf{D}}^{(p,v,w)}\right)^T \hat{\mathbf{D}}^{(p,v,w)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \left(\hat{\mathbf{D}}^{(p,v,w)}\right)^T \hat{\mathbf{D}}^{(p,v,w)} \end{bmatrix}. \tag{77}$$

Upon substituting Eqs. (73)–(77) into Eqs. (68) and (69), one obtains

$$\left(\mathbf{M}^k + \mathbf{K}^k\right) \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{U}_k + \mathbf{S}^k \mathbf{A} \mathbf{U}_k - b\, \mathbf{S}^k \mathbf{Q}_k = \int_{\mathbf{\Gamma}_k} \left[\left(\left(\mathbf{a}\, u_k^D - b\, \mathbf{q}_k^D\right) - (\mathbf{a}\, u - b\, \mathbf{q})^{\star}\right) \cdot \mathbf{n}\right] \mathbf{L}\, d\mathbf{\Gamma}_k, \tag{78}$$

$$\left(\mathcal{M}^k + \mathcal{K}^k\right) \mathbf{Q}_k - \mathcal{S}^k \mathbf{U}_k = -\int_{\mathbf{\Gamma}_k} \left(u_k^D - u^{\star}\right) \mathbf{N} \mathbf{L}\, d\mathbf{\Gamma}_k. \tag{79}$$

One may now define 'modified mass matrices' as follows

$$\widetilde{\mathbf{M}}^k \equiv \left(\mathbf{M}^k + \mathbf{K}^k\right), \tag{80}$$

$$\widetilde{\mathcal{M}}^k \equiv \left(\mathcal{M}^k + \mathcal{K}^k\right), \tag{81}$$

where $\widetilde{\mathbf{M}}^k$ and $\widetilde{\mathcal{M}}^k$ are guaranteed to be symmetric positive-definite provided that $\mathbf{K}^k$ and $\mathcal{K}^k$ are symmetric positive-semidefinite. Note that if one requires that $c_{vw} \geq 0$ and $\kappa_{vw} \geq 0$, then $\mathbf{K}^k$ and $\mathcal{K}^k$ are (in fact) symmetric positive-semidefinite.

On substituting Eqs. (80) and (81) into Eqs. (78) and (79), one obtains Eqs. (58) and (59). This completes the proof of Lemma 3.3. □

Theorem 3.1 *If the VCJH schemes (for which Lemmas 3.1–3.3 hold) are employed in conjunction with the Lax–Friedrichs formulation [14,28] for the advective numerical flux* $\mathbf{f}^{\star}_{adv}$

$$\mathbf{f}^{\star}_{adv} = (\mathbf{a}\, u)^{\star} = \{\{\mathbf{a}\, u^D\}\} + \frac{\lambda}{2} |\mathbf{a} \cdot \mathbf{n}| \, [\![u^D]\!], \tag{82}$$

for which $0 \leq \lambda \leq 1$ *is an upwinding parameter,* $\{\{\cdot\}\}$ *is an averaging operator,* $[\![\cdot]\!]$ *is a differencing (jump) operator, and the LDG formulation [12] for the common numerical solution* $u^{\star}$ *and diffusive numerical flux* $\mathbf{f}^{\star}_{dif}$

$$u^{\star} = \{\{u^D\}\} - \beta \cdot [\![u^D]\!], \tag{83}$$

$$\mathbf{f}^{\star}_{dif} = (b\, \mathbf{q})^{\star} = \{\{b\, \mathbf{q}^D\}\} + \tau [\![u^D]\!] + \beta\, b [\![\mathbf{q}^D]\!], \tag{84}$$

for which $\beta = (\beta_x, \beta_y, \beta_z) = (\beta_1, \beta_2, \beta_3)$ *is a directional parameter and* $\tau \geq 0$ *is a penalty parameter, then it can be shown that the following result holds*

$$\sum_{k=1}^{N} \left(\frac{\mathrm{d}}{\mathrm{d}t} \|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}\right) \leq 0. \tag{85}$$

Proof Consider multiplying Eq. (58) on the left by $\mathbf{U}_k^T$ and Eq. (59) on the left by $\mathbf{Q}_k^T$ in order to obtain

$$\mathbf{U}_k^T\,\widetilde{\mathbf{M}}^k\,\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k+\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{A}\mathbf{U}_k-b\,\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{Q}_k=\int\limits_{\boldsymbol{\Gamma}_k}\left[\left(\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)-(\mathbf{a}\,u-b\,\mathbf{q})^\star\right)\cdot\mathbf{n}\right]u_k^D\;d\boldsymbol{\Gamma}_k, \tag{86}$$

$$\mathbf{Q}_k^T\,\widetilde{\mathcal{M}}^k\mathbf{Q}_k-\mathbf{Q}_k^T\,\mathcal{S}^k\mathbf{U}_k=-\int\limits_{\boldsymbol{\Gamma}_k}\left(u_k^D-u^\star\right)\left(\mathbf{q}_k^D\cdot\mathbf{n}\right)\,d\boldsymbol{\Gamma}_k, \tag{87}$$

where the fact that $u_k^D=\mathbf{U}_k^T\,\mathbf{L}$ and $\mathbf{q}_k^D\cdot\mathbf{n}=\mathbf{Q}_k^T\,\mathbf{N}\mathbf{L}$ has been used. Equations (86) and (87) can be simplified by introducing the following identities

$$\mathbf{U}_k^T\,\widetilde{\mathbf{M}}^k\,\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{U}_k^T\,\widetilde{\mathbf{M}}^k\mathbf{U}_k\right)=\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|_{\widetilde{\mathbf{M}}}^2, \tag{88}$$

$$\mathbf{Q}_k^T\,\widetilde{\mathcal{M}}^k\mathbf{Q}_k=\|\mathbf{Q}_k\|_{\widetilde{\mathcal{M}}}^2, \tag{89}$$

where, because $\widetilde{\mathbf{M}}^k$ and $\widetilde{\mathcal{M}}^k$ are symmetric positive-definite matrices, $\|\mathbf{U}_k\|_{\widetilde{\mathbf{M}}}$ and $\|\mathbf{Q}_k\|_{\widetilde{\mathcal{M}}}$ are norms. Upon using Eqs. (88) and (89) to simplify Eqs. (86) and (87), one obtains

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|_{\widetilde{\mathbf{M}}}^2+\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{A}\mathbf{U}_k-b\,\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{Q}_k=\int\limits_{\boldsymbol{\Gamma}_k}\left[\left(\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)-(\mathbf{a}\,u-b\,\mathbf{q})^\star\right)\cdot\mathbf{n}\right]u_k^D\;d\boldsymbol{\Gamma}_k, \tag{90}$$

$$\|\mathbf{Q}_k\|_{\widetilde{\mathcal{M}}}^2-\mathbf{Q}_k^T\,\mathcal{S}^k\mathbf{U}_k=-\int\limits_{\boldsymbol{\Gamma}_k}\left(u_k^D-u^\star\right)\left(\mathbf{q}_k^D\cdot\mathbf{n}\right)\,d\boldsymbol{\Gamma}_k. \tag{91}$$

One may now multiply Eq. (91) by b and add the result to Eq. (90) in order to obtain

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|_{\widetilde{\mathbf{M}}}^2+b\,\|\mathbf{Q}_k\|_{\widetilde{\mathcal{M}}}^2+\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{A}\mathbf{U}_k-b\left(\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{Q}_k+\mathbf{Q}_k^T\mathcal{S}^k\mathbf{U}_k\right)\\&=\int\limits_{\boldsymbol{\Gamma}_k}\left[\left(\left(\mathbf{a}\,u_k^D-b\,\mathbf{q}_k^D\right)-(\mathbf{a}\,u-b\,\mathbf{q})^\star\right)\cdot\mathbf{n}\right]u_k^D\;d\boldsymbol{\Gamma}_k-b\int\limits_{\boldsymbol{\Gamma}_k}\left(u_k^D-u^\star\right)\left(\mathbf{q}_k^D\cdot\mathbf{n}\right)\,d\boldsymbol{\Gamma}_k.\end{aligned} \tag{92}$$

Equation (92) can be simplified by noting that

$$\begin{aligned}&\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{A}\mathbf{U}_k\\&=\int\limits_{\boldsymbol{\Omega}_k}u_k^D\,\nabla\cdot\left(\mathbf{a}u_k^D\right)\,d\boldsymbol{\Omega}_k=\frac{1}{2}\int\limits_{\boldsymbol{\Omega}_k}\nabla\cdot\left(\mathbf{a}\left(u_k^D\right)^2\right)\,d\boldsymbol{\Omega}_k=\frac{1}{2}\int\limits_{\boldsymbol{\Gamma}_k}\left(u_k^D\right)^2(\mathbf{a}\cdot\mathbf{n})\;d\boldsymbol{\Gamma}_k,\end{aligned} \tag{93}$$

and that

$$\mathbf{U}_k^T\,\mathbf{S}^k\mathbf{Q}_k+\mathbf{Q}_k^T\mathcal{S}^k\mathbf{U}_k=\int\limits_{\boldsymbol{\Omega}_k}\left(u_k^D\left(\nabla\cdot\mathbf{q}_k^D\right)+\mathbf{q}_k^D\cdot\nabla u_k^D\right)\,d\boldsymbol{\Omega}_k=\int\limits_{\boldsymbol{\Gamma}_k}u_k^D\left(\mathbf{q}_k^D\cdot\mathbf{n}\right)\,d\boldsymbol{\Gamma}_k. \tag{94}$$

Upon substituting Eqs. (93) and (94) into Eq. (92) and rearranging the result, one obtains

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}} + b\,\|\mathbf{Q}_k\|^2_{\widetilde{\mathcal{M}}} &= \int\limits_{\boldsymbol{\Gamma}_k}\left[u_k^D\left(\left(\frac{\mathbf{a}\,u_k^D}{2} - b\,\mathbf{q}_k^D\right) - (\mathbf{a}\,u - b\,\mathbf{q})^\star\right) + b\,u^\star\mathbf{q}_k^D\right]\cdot\mathbf{n}\;d\boldsymbol{\Gamma}_k\\ &= \int\limits_{\boldsymbol{\Gamma}_k}\left[u_k^D\left(\frac{\mathbf{a}\,u_k^D}{2} - (\mathbf{a}\,u)^\star\right) - u_k^D\left(b\,\mathbf{q}_k^D - (b\,\mathbf{q})^\star\right) + b\,u^\star\mathbf{q}_k^D\right]\cdot\mathbf{n}\;d\boldsymbol{\Gamma}_k, \qquad (95)\end{aligned}$$

where the fact that $(\mathbf{a}\,u - b\,\mathbf{q})^\star = (\mathbf{a}\,u)^\star - (b\,\mathbf{q})^\star$ has been used. Next, upon summing Eq. (95) over all elements in the mesh, one obtains

$$\begin{aligned}\frac{1}{2}\sum_{k=1}^{N}\left(\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}\right) &= -b\sum_{k=1}^{N}\|\mathbf{Q}_k\|^2_{\widetilde{\mathcal{M}}}\\ &+\sum_{k=1}^{N}\left\{\int\limits_{\boldsymbol{\Gamma}_k}\left[u_k^D\left(\frac{\mathbf{a}\,u_k^D}{2} - (\mathbf{a}\,u)^\star\right) - u_k^D\left(b\,\mathbf{q}_k^D - (b\,\mathbf{q})^\star\right) + b\,u^\star\mathbf{q}_k^D\right]\cdot\mathbf{n}\;d\boldsymbol{\Gamma}_k\right\}. \qquad (96)\end{aligned}$$

In order to demonstrate that the VCJH schemes are stable (in accordance with Eq. (34)), one must show that the right hand side (RHS) of Eq. (96) is non-positive. The first term on the RHS of Eq. (96) is clearly non-positive, however, the second term on the RHS has an ambiguous sign, and is only assured to be non-positive for appropriate formulations of the numerical fluxes $(\mathbf{a}\,u)^\star$ and $(b\,\mathbf{q})^\star$, and the common numerical solution $u^\star$. The Lax–Friedrichs approach [14,28] is a well-known approach for treating the advective numerical flux $(\mathbf{a}\,u)^\star$ and the Central Flux (CF) [5,19], Bassi Rebay 1 (BR1) [5], Bassi Rebay 2 (BR2) [6], Local Discontinuous Galerkin (LDG) [12], Compact Discontinuous Galerkin (CDG) [30], and Interior Penalty (IP) [2] approaches are well-known approaches for treating the diffusive numerical flux $(b\,\mathbf{q})^\star$ and the common numerical solution $u^\star$. For the sake of brevity, the remainder of this discussion will not consider all the different possible combinations of advective and diffusive flux formulations. Rather, for illustrative purposes, it will be shown that a combination of the Lax–Friedrichs and LDG flux formulations ensures that the second term on the RHS of Eq. (96) is non-positive.

Consider the normal component of the Lax–Friedrichs advective numerical flux which takes the form

$$(\mathbf{a}\,u)^\star\cdot\mathbf{n} = \left(\{\{\mathbf{a}\,u^D\}\} + \frac{\lambda}{2}|\mathbf{a}\cdot\mathbf{n}|\;[\![u^D]\!]\right)\cdot\mathbf{n}, \qquad (97)$$

where λ is a directional parameter which yields an upwind biased flux for $\lambda > 0$, and $\{\{\cdot\}\}$ and $[\![\cdot]\!]$ are average and jump operators defined such that

$$\{\{\mathbf{a}\,u^D\}\} = \{\{u^D\}\}\mathbf{a} = \frac{1}{2}\left(u_{k_-}^D + u_{k_+}^D\right)\mathbf{a}, \qquad [\![u^D]\!] = u_{k_-}^D\mathbf{n}_- + u_{k_+}^D\mathbf{n}_+, \qquad (98)$$

where $u_{k_-}^D$ and $\mathbf{n}_-$ represent the solution and normal vector which belong to the k^{th} element and $u_{k_+}^D$ and $\mathbf{n}_+$ represent the solutions and normal vectors which belong to adjoining elements. Upon substituting Eq. (98) into Eq. (97) and noting that $\mathbf{n}\equiv\mathbf{n}_-$, one obtains

$$(\mathbf{a}\,u)^\star\cdot\mathbf{n} = \frac{1}{2}\left(u_{k_-}^D + u_{k_+}^D\right)(\mathbf{a}\cdot\mathbf{n}) + \frac{\lambda}{2}|\mathbf{a}\cdot\mathbf{n}|\left(u_{k_-}^D - u_{k_+}^D\right). \qquad (99)$$

Next, one may consider the LDG common numerical solution which takes the form

$$u^{\star} = \{\{u^D\}\} - \beta \cdot [\![u^D]\!] \\ = \frac{1}{2}\left(u^D_{k_-} + u^D_{k_+}\right) - \left(u^D_{k_-} - u^D_{k_+}\right)(\beta \cdot \mathbf{n}), \tag{100}$$

and the normal component of the LDG diffusive numerical flux which takes the form

$$(b\,\mathbf{q})^{\star} \cdot \mathbf{n} = \left(\{\{b\,\mathbf{q}^D\}\} + \tau[\![u^D]\!] + \beta\, b[\![\mathbf{q}^D]\!]\right) \cdot \mathbf{n} \\ = b\left(\frac{1}{2}\left(\mathbf{q}^D_{k_-} + \mathbf{q}^D_{k_+}\right) + \left(\mathbf{q}^D_{k_-} - \mathbf{q}^D_{k_+}\right)(\beta \cdot \mathbf{n})\right) \cdot \mathbf{n} + \tau\left(u^D_{k_-} - u^D_{k_+}\right), \tag{101}$$

where $\{\{b\,\mathbf{q}^D\}\}$ and $[\![\mathbf{q}^D]\!]$ have been defined such that

$$\{\{b\,\mathbf{q}^D\}\} = \{\{\mathbf{q}^D\}\}b = \frac{1}{2}\left(\mathbf{q}^D_{k_-} + \mathbf{q}^D_{k_+}\right)b, \qquad [\![\mathbf{q}^D]\!] = \mathbf{q}^D_{k_-} - \mathbf{q}^D_{k_+}. \tag{102}$$

In Eqs. (100) and (101), β is a directional parameter which biases the solution and the auxiliary variable in opposite directions (if one is biased upwind the other is biased downwind and vice versa), τ is a penalty parameter which controls jumps in the solution, $\mathbf{q}^D_{k_-}$ denotes the auxiliary variable which belongs to the k^{th} element, and $\mathbf{q}^D_{k_+}$ denotes the auxiliary variables which belong to adjoining elements.

Upon substituting Eqs. (99), (100), and (101) into Eq. (96) and replacing u^D_k and $\mathbf{q}^D_k$ with $u^D_{k_-}$ and $\mathbf{q}^D_{k_-}$, respectively, one obtains an expression of the form

$$\frac{1}{2}\sum_{k=1}^{N}\left(\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}\right) \\ = -b\sum_{k=1}^{N}\|\mathbf{Q}_k\|^2_{\widetilde{\mathcal{M}}} + \sum_{k=1}^{N}\left\{\int_{\mathbf{\Gamma}_k}\left[u^D_{k_-}\left(\frac{u^D_{k_+}}{2}(\mathbf{a}\cdot\mathbf{n}) - \frac{\lambda}{2}|\mathbf{a}\cdot\mathbf{n}|\left(u^D_{k_-} - u^D_{k_+}\right)\right)\right.\right. \\ -u^D_{k_-}\left(b\,\mathbf{q}^D_{k_-}\cdot\mathbf{n} - b\left(\frac{1}{2}\left(\mathbf{q}^D_{k_-} + \mathbf{q}^D_{k_+}\right) + \left(\mathbf{q}^D_{k_-} - \mathbf{q}^D_{k_+}\right)(\beta\cdot\mathbf{n})\right)\cdot\mathbf{n} - \tau\left(u^D_{k_-} - u^D_{k_+}\right)\right) \\ \left.\left. +b\left(\frac{1}{2}\left(u^D_{k_-} + u^D_{k_+}\right) - \left(u^D_{k_-} - u^D_{k_+}\right)(\beta\cdot\mathbf{n})\right)\mathbf{q}^D_{k_-}\cdot\mathbf{n}\right]d\mathbf{\Gamma}_k\right\}. \tag{103}$$

One may simplify Eq. (103) by replacing the summation over elements in the mesh (applied to the second term on the RHS) with a summation over faces (f) in the mesh. Thereafter, upon assuming periodic boundary conditions and canceling like terms, one obtains

$$\frac{1}{2}\sum_{k=1}^{N}\left(\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}\right) \\ = -b\sum_{k=1}^{N}\|\mathbf{Q}_k\|^2_{\widetilde{\mathcal{M}}} - \sum_{f=1}^{N_f}\left\{\int_{\mathbf{\Gamma}_f}\left[\left(\frac{\lambda}{2}|\mathbf{a}\cdot\mathbf{n}| + \tau\right)\left(u^D_{f_-} - u^D_{f_+}\right)^2\right]d\mathbf{\Gamma}_f\right\}, \tag{104}$$

where N_f is the total number of faces in the mesh and $u^D_{f_-}$ and $u^D_{f_+}$ are the solutions on opposite sides of face f. Finally, because $b \geq 0$, $\lambda \geq 0$, and $\tau \geq 0$, the terms on the RHS of

Eq. (104) are non-positive and it follows that

$$\frac{1}{2}\sum_{k=1}^{N}\left(\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{U}_k\|^2_{\widetilde{\mathbf{M}}}\right) \leq 0. \tag{105}$$

This completes the proof of theorem 3.1. □

Remark In summary, the stability of a class of FR schemes (the VCJH schemes) has been proven under the following assumptions:

- The flux is a linear advective-diffusive flux.
- The advection–diffusion problem is discretized on straight-sided tetrahedra $\mathbf{\Omega}_k$, for which $J_k = const$, $J_k > 0$, and Eqs. (10)–(16) hold.
- The divergence of the flux correction $\hat{\nabla}\cdot\hat{\mathbf{f}}^C$ in reference space (Eq. (28)) is defined using a VCJH correction field $\phi_{f,l} = \hat{\nabla}\cdot\mathbf{h}_{f,l}$ parameterized by constant coefficients c_{vw}, such that Eq. (43) holds.
- The gradient of the solution correction $\hat{\nabla}\hat{u}^C$ in reference space (Eq. (22)) is defined using a VCJH correction field $\psi_{f,l} = \hat{\nabla}\cdot\mathbf{g}_{f,l}$ parameterized by constant coefficients κ_{vw}, such that Eq. (53) holds.
- The coefficients of parameterization are non-negative (i.e. $c_{vw} \geq 0$ and $\kappa_{vw} \geq 0$) ensuring that the modified mass matrices $\widetilde{\mathbf{M}}^k$ and $\widetilde{\mathcal{M}}^k$ are symmetric positive-definite and that $\|\mathbf{U}_k\|_{\widetilde{\mathbf{M}}}$ and $\|\mathbf{Q}_k\|_{\widetilde{\mathcal{M}}}$ are norms.
- The advective numerical flux is computed using the Lax–Friedrichs approach (Eq. (99)).
- The diffusive numerical flux and common numerical solution are computed using the LDG approach (Eqs. (100) and (101)).

Finally, note that stability has been proven for all orders of accuracy $p \geq 0$, independent of the locations of solution points $\hat{\mathbf{x}}_i$ and flux points $\hat{\mathbf{x}}_{f,l}$.

4 Choosing the Parameterizing Coefficients for the VCJH Schemes

Thus far, there has not been a discussion of the precise approach for selecting the coefficients c_{vw} and κ_{vw} for parameterizing the VCJH correction functions and fields. In particular, the previous section demonstrated that only loose constraints on c_{vw} and κ_{vw} are required to ensure stability, as it was shown that choosing $c_{vw} \geq 0$ and $\kappa_{vw} \geq 0$ results in a class of energy stable FR schemes (the VCJH schemes). This section will propose an additional set of constraints on c_{vw} and κ_{vw} based on symmetry considerations, and thereby provide a more explicit approach for selecting the coefficients.

4.1 Symmetry Considerations Pertaining to Derivative Operators

It is important to ensure that the derivative operators used in the formulation of the VCJH schemes are symmetric. In particular, it is necessary to ensure that the operators are directionally unbiased so as to avoid introducing artificial asymmetries into simulations of (potentially) symmetric physical phenomenon. Towards this end, one may impose constraints on the coefficients c_{vw} and κ_{vw} in order to ensure that the operators are symmetric.

4.1.1 Preliminaries

In order to begin the process of identifying constraints on the coefficients, one must first examine the precise form of the derivative operators used in the formulation of the VCJH schemes. Towards this end, consider the 'VCJH derivative operators' of degree p which take the following form

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\,\hat{D}^{(p,v,w)}(f)\,\hat{D}^{(p,v,w)}(g)\,, \tag{106}$$

and

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} \kappa_{vw}\,\hat{D}^{(p,v,w)}(\mathcal{F})\cdot\hat{D}^{(p,v,w)}(\mathcal{G})\,, \tag{107}$$

where f and g are arbitrary, continuous, p times differentiable, scalar-valued functions, and $\mathcal{F}$ and $\mathcal{G}$ are arbitrary, continuous, p times differentiable, vector-valued functions. The derivative operators in Eqs. (106) and (107) were used in the formulation of the VCJH schemes, and (more precisely) in the context of Eqs. (43) and (53), respectively. In particular, Eq. (43) contains the derivative operator defined in Eq. (106), with functions f and g replaced by functions $\hat{\nabla}\cdot\hat{\mathbf{f}}^C$ and $\hat{\ell}_j$, respectively. Furthermore, Eq. (53) contains the derivative operator defined in Eq. (107), with functions $\mathcal{F}$ and $\mathcal{G}$ replaced by functions $\hat{\nabla}\hat{u}^C$ and $\hat{\mathcal{L}}_{\hat{m},j}$, respectively.

Next, in order to evaluate the symmetry of the VCJH derivative operators, it is useful to rewrite them in quadratic form. The quadratic form of a generic derivative operator $\hat{D}(f)\,\hat{D}(g)$ can be obtained by substituting f in place of g in order to obtain

$$\hat{D}(f)\,\hat{D}(f) = \left(\hat{D}(f)\right)^2. \tag{108}$$

Similarly, the quadratic form of a generic derivative operator $\hat{D}(\mathcal{F})\cdot\hat{D}(\mathcal{G})$ can be obtained by substituting $\mathcal{F}$ in place of $\mathcal{G}$ in order to obtain

$$\hat{D}(\mathcal{F})\cdot\hat{D}(\mathcal{F})\,. \tag{109}$$

In following this procedure, one may substitute f in place of g in Eq. (106) and $\mathcal{F}$ in place of $\mathcal{G}$ in Eq. (107), in order to obtain the following quadratic forms of the VCJH derivative operators

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\left(\hat{D}^{(p,v,w)}(f)\right)^2, \tag{110}$$

and

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} \kappa_{vw}\,\hat{D}^{(p,v,w)}(\mathcal{F})\cdot\hat{D}^{(p,v,w)}(\mathcal{F})\,. \tag{111}$$

The VCJH operators in Eqs. (110) and (111) are now in a form that can be conveniently analyzed. In particular, well-known 'operator theory', (a good review of which appears in [7, 13], and chapter 6 of [16]), can now be used to determine constraints on the VCJH operators that will ensure their symmetry.

In what follows, operator theory will be used to construct a general, symmetric operator of degree p and thereafter this symmetric operator will be compared to the operators in Eqs. (110) and (111) in order to arrive at a set of constraints on c_{vw} and κ_{vw}.

4.1.2 Theory for Constructing a Symmetric Derivative Operator

In order to construct a general symmetric derivative operator of degree p, one may first consider the general quadratic form for a derivative operator of degree p

$$(\Delta f)^T \, \mathbf{C} \, (\Delta f) \,, \tag{112}$$

where $\Delta f \in \mathbb{R}^{d^p}$ is a vector containing the p^{th} degree derivatives of the function f, d is the number of spatial dimensions, and $\mathbf{C} \in \mathbb{R}^{d^p \times d^p}$ is a symmetric matrix containing at most $d^p(d^p+1)/2$ unique entries. For $d = 3$ and $p = 2$, Δf takes the following form

$$\Delta f = \left[\frac{\partial^2 f}{\partial \hat{x}^2}, \; \frac{\partial^2 f}{\partial \hat{y}^2}, \; \frac{\partial^2 f}{\partial \hat{z}^2}, \; \frac{\partial^2 f}{\partial \hat{x} \partial \hat{y}}, \; \frac{\partial^2 f}{\partial \hat{y} \partial \hat{x}}, \; \frac{\partial^2 f}{\partial \hat{x} \partial \hat{z}}, \; \frac{\partial^2 f}{\partial \hat{z} \partial \hat{x}}, \; \frac{\partial^2 f}{\partial \hat{y} \partial \hat{z}}, \; \frac{\partial^2 f}{\partial \hat{z} \partial \hat{y}} \right]^T, \tag{113}$$

where it is important to note that although derivatives such as $\frac{\partial^2 f}{\partial \hat{x} \partial \hat{y}}$ and $\frac{\partial^2 f}{\partial \hat{y} \partial \hat{x}}$ are identical for continuous functions, for now they will be treated distinctly in order to simplify the analysis (as recommended in [7]).

According to operator theory, a derivative operator is defined to be 'symmetric' if it is invariant under orthogonal transformations of the space, i.e. rotations and reflections of the coordinate system [7,16]. The operator in Eq. (112) is invariant under orthogonal transformations if and only if it satisfies the following condition

$$(\mathbf{R} \Delta f)^T \, \mathbf{C} \, (\mathbf{R} \Delta f) = (\Delta f)^T \, \mathbf{C} \, (\Delta f) \,, \tag{114}$$

where $\mathbf{R} \in \mathbb{R}^{d^p \times d^p}$ is an arbitrary orthogonal matrix. Upon manipulating Eq. (114) and noting that $\mathbf{R}^T = \mathbf{R}^{-1}$, one obtains the following equivalent condition

$$\mathbf{R}^T \mathbf{C} = \mathbf{C} \, \mathbf{R}^T. \tag{115}$$

An obvious choice of $\mathbf{C}$ which satisfies Eq. (115) (and to the authors' knowledge the only choice for general $\mathbf{R}$) is $\mathbf{C} = c\mathbf{I}$ where c is an arbitrary scalar, and $\mathbf{I}$ is the identity matrix in $\mathbb{R}^{d^p \times d^p}$. Upon substituting this choice of $\mathbf{C}$ into Eq. (112), one obtains the following derivative operator

$$c \, (\Delta f)^T \, (\Delta f) \,. \tag{116}$$

Next, one may reformulate Eq. (116) by expanding the inner product $(\Delta f)^T \, (\Delta f)$ and then combining all resulting non-distinct derivative terms (such as the terms $c \left(\frac{\partial^2 f}{\partial \hat{x} \partial \hat{y}} \right)^2$ and $c \left(\frac{\partial^2 f}{\partial \hat{y} \partial \hat{x}} \right)^2$ which arise in Eq. (116) when $d = 3$ and $p = 2$). For example, if Δf is given by Eq. (113), then Eq. (116) becomes

$$
\begin{aligned}
c\,(\Delta f)^T\,(\Delta f) = c\Bigg\{&\left(\frac{\partial^2 f}{\partial \hat{x}^2}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{y}^2}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{z}^2}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{x}\partial \hat{y}}\right)^2\\
&+\left(\frac{\partial^2 f}{\partial \hat{y}\partial \hat{x}}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{x}\partial \hat{z}}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{z}\partial \hat{x}}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{y}\partial \hat{z}}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{z}\partial \hat{y}}\right)^2\Bigg\}\\
= c\Bigg\{&\left(\frac{\partial^2 f}{\partial \hat{x}^2}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{y}^2}\right)^2+\left(\frac{\partial^2 f}{\partial \hat{z}^2}\right)^2\\
&+2\left(\frac{\partial^2 f}{\partial \hat{x}\partial \hat{y}}\right)^2+2\left(\frac{\partial^2 f}{\partial \hat{x}\partial \hat{z}}\right)^2+2\left(\frac{\partial^2 f}{\partial \hat{y}\partial \hat{z}}\right)^2\Bigg\}.
\end{aligned} \tag{117}
$$

For the more general case of $d = 3$ and arbitrary p, there are a total of

$$
\binom{p}{v-1}\binom{v-1}{w-1}, \tag{118}
$$

non-distinct terms associated with the p^{th} degree derivative term that takes the form

$$
c\left(\frac{\partial^p f}{\partial \hat{x}^{(p-v+1)}\partial \hat{y}^{(v-w)}\partial \hat{z}^{(w-1)}}\right)^2, \tag{119}
$$

where $v = 1, \ldots, p$ and $w = 1, \ldots, v$. It is interesting to note that Eq. (118) contains an expression for the p^{th} degree trinomial coefficients (the coefficients on the p^{th} degree terms in the expansion of $\left(\hat{x}+\hat{y}+\hat{z}\right)^p$).

On combining all non-distinct terms for the operator in Eq. (116), for the case of $d = 3$, one obtains

$$
c\,(\Delta f)^T\,(\Delta f) = c\sum_{v=1}^{p+1}\sum_{w=1}^{v}\binom{p}{v-1}\binom{v-1}{w-1}\left(\frac{\partial^p f}{\partial \hat{x}^{(p-v+1)}\partial \hat{y}^{(v-w)}\partial \hat{z}^{(w-1)}}\right)^2, \tag{120}
$$

which is the generalization of Eq. (117) for arbitrary p. On substituting Eq. (37) into Eq. (120), one obtains

$$
c\sum_{v=1}^{p+1}\sum_{w=1}^{v}\binom{p}{v-1}\binom{v-1}{w-1}\left(\hat{D}^{(p,v,w)}(f)\right)^2. \tag{121}
$$

Equation (121) contains a final, convenient formulation for a p^{th} degree derivative operator that is invariant under orthogonal transformations in 3D.

4.2 Defining the Coefficients

In order to obtain appropriate definitions for the coefficients c_{vw} and κ_{vw}, one may compare the derivative operator in Eq. (121) to the derivative operators in Eqs. (110) and (111). Upon comparing Eqs. (110) and (121), one obtains the following expression for each coefficient c_{vw}

$$
c_{vw} = c\binom{p}{v-1}\binom{v-1}{w-1}, \tag{122}
$$

where in order to ensure that $c_{vw} \geq 0$, one requires that $c \geq 0$.

Next, in order to define each coefficient κ_{vw}, one must first substitute the component-wise definition of $\mathcal{F}$ (i.e. $\mathcal{F} = \left(\mathcal{F}_{\hat{x}}, \mathcal{F}_{\hat{y}}, \mathcal{F}_{\hat{z}}\right) = \left(\mathcal{F}_{\hat{1}}, \mathcal{F}_{\hat{2}}, \mathcal{F}_{\hat{3}}\right)$) into Eq. (111), as follows

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} \kappa_{vw} \hat{D}^{(p,v,w)}\left(\mathcal{F}\right) \cdot \hat{D}^{(p,v,w)}\left(\mathcal{F}\right)$$
$$= \sum_{v=1}^{p+1}\sum_{w=1}^{v} \kappa_{vw} \left[\left(\hat{D}^{(p,v,w)}\left(\mathcal{F}_{\hat{1}}\right)\right)^2 + \left(\hat{D}^{(p,v,w)}\left(\mathcal{F}_{\hat{2}}\right)\right)^2 + \left(\hat{D}^{(p,v,w)}\left(\mathcal{F}_{\hat{3}}\right)\right)^2\right]. \tag{123}$$

Next, setting Eq. (123) aside for the moment, consider modifying Eq. (121) by replacing c with an arbitrary coefficient κ and replacing f with the $\hat{m}^{th}$ component of $\mathcal{F}$ as follows

$$\kappa \sum_{v=1}^{p+1}\sum_{w=1}^{v} \binom{p}{v-1}\binom{v-1}{w-1} \left(\hat{D}^{(p,v,w)}\left(\mathcal{F}_{\hat{m}}\right)\right)^2, \qquad \hat{m} = \hat{1}, \hat{2}, \hat{3}. \tag{124}$$

On comparing Eq. (124) to Eq. (123), one obtains the following expression for each coefficient κ_{vw}

$$\kappa_{vw} = \kappa \binom{p}{v-1}\binom{v-1}{w-1}, \tag{125}$$

where in order to ensure that $\kappa_{vw} \geq 0$, one requires that $\kappa \geq 0$.

In summary, if the coefficients c_{vw} and κ_{vw} are chosen in accordance with Eqs. (122) and (125), one obtains derivative operators for each scheme which preserve physical symmetry in the sense that they are invariant under orthogonal transformations of the coordinate system. Furthermore, the resulting 'symmetry-preserving' schemes are straightforwardly defined in terms of two parameters, c and κ, and are guaranteed to be stable for all choices of $c \geq 0$ and $\kappa \geq 0$.

5 Equivalence of VCJH Schemes and Certain Filtered DG Schemes

In this section, it will be shown that, for all choices of $c \geq 0$ and $\kappa \geq 0$, the class of VCJH schemes is equivalent to a class of filtered, collocation-based, nodal DG schemes. The equivalence of VCJH schemes with certain filtered DG schemes has been shown for 1D linear advection problems by Allaneau and Jameson [1]. In what follows, this result will be extended to the case of 3D advection–diffusion problems on tetrahedral elements.

In order to begin demonstrating the equivalence of the VCJH schemes and certain collocation-based, nodal DG schemes, one must first examine the formulation of the *unfiltered*, collocation-based, nodal DG scheme. For the linear advection–diffusion problem, this scheme can be shown to take the following form

$$\mathbf{M}^k \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k + \mathbf{S}^k \mathbf{A}\mathbf{U}_k - b\,\mathbf{S}^k\mathbf{Q}_k = \int_{\mathbf{\Gamma}_k} \left[\left(\left(\mathbf{a}\,u_k^D - b\,\mathbf{q}_k^D\right) - \left(\mathbf{a}\,u - b\,\mathbf{q}\right)^{\star}\right)\cdot \mathbf{n}\right] \mathbf{L}\, d\mathbf{\Gamma}_k, \tag{126}$$

$$\mathcal{M}^k\,\mathbf{Q}_k - \mathcal{S}^k\mathbf{U}_k = -\int_{\mathbf{\Gamma}_k} \left(u_k^D - u^{\star}\right) \mathbf{N}\mathbf{L}\, d\mathbf{\Gamma}_k. \tag{127}$$

The derivation of this result is omitted for the sake of brevity. Consider simplifying Eqs. (126) and (127) by introducing the following abbreviations

$$\mathbf{RHS}_{DG1} \equiv \int_{\boldsymbol{\Gamma}_k} \left[\left(\left(\mathbf{a}\, u_k^D - b\, \mathbf{q}_k^D \right) - (\mathbf{a}\, u - b\, \mathbf{q})^{\star} \right) \cdot \mathbf{n} \right] \mathbf{L}\; d\boldsymbol{\Gamma}_k, \tag{128}$$

$$\mathbf{RHS}_{DG2} \equiv - \int_{\boldsymbol{\Gamma}_k} \left(u_k^D - u^{\star} \right) \mathbf{NL}\; d\boldsymbol{\Gamma}_k. \tag{129}$$

Upon substituting Eqs. (128) and (129) into Eqs. (126) and (127) and rearranging the result, one obtains

$$\mathbf{M}^k \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k = -\mathbf{S}^k \mathbf{A} \mathbf{U}_k + b\, \mathbf{S}^k \mathbf{Q}_k + \mathbf{RHS}_{DG1}, \tag{130}$$

$$\mathcal{M}^k \mathbf{Q}_k = \mathcal{S}^k \mathbf{U}_k + \mathbf{RHS}_{DG2}. \tag{131}$$

On multiplying Eq. (130) by $\left(\mathbf{M}^k\right)^{-1}$ and Eq. (131) by $\left(\mathcal{M}^k\right)^{-1}$, one obtains the DG residual $\mathbf{R}_{DG}$ and auxiliary variable $\mathbf{Q}_{DG}$

$$\mathbf{R}_{DG} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k = \left(\mathbf{M}^k\right)^{-1} \left(-\mathbf{S}^k \mathbf{A} \mathbf{U}_k + b\, \mathbf{S}^k \mathbf{Q}_k + \mathbf{RHS}_{DG1} \right), \tag{132}$$

$$\mathbf{Q}_{DG} \equiv \mathbf{Q}_k = \left(\mathcal{M}^k\right)^{-1} \left(\mathcal{S}^k \mathbf{U}_k + \mathbf{RHS}_{DG2} \right). \tag{133}$$

Having obtained a simplified formulation of the collocation-based nodal DG scheme (Eqs. (132) and (133)), one may compare it to a simplified formulation of the VCJH schemes (which can be obtained from Eqs. (58) and (59)). Towards this end, consider substituting Eqs. (128) and (129) into Eqs. (58) and (59) and rearranging the result in order to obtain

$$\widetilde{\mathbf{M}}^k \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k = -\mathbf{S}^k \mathbf{A} \mathbf{U}_k + b\, \mathbf{S}^k \mathbf{Q}_k + \mathbf{RHS}_{DG1}, \tag{134}$$

$$\widetilde{\mathcal{M}}^k \mathbf{Q}_k = \mathcal{S}^k \mathbf{U}_k + \mathbf{RHS}_{DG2}. \tag{135}$$

On multiplying Eq. (134) by $\left(\widetilde{\mathbf{M}}^k\right)^{-1}$ and Eq. (135) by $\left(\widetilde{\mathcal{M}}^k\right)^{-1}$, one obtains the VCJH residual $\mathbf{R}_{VCJH}$ and auxiliary variable $\mathbf{Q}_{VCJH}$

$$\mathbf{R}_{VCJH} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{U}_k = \left(\widetilde{\mathbf{M}}^k\right)^{-1} \left(-\mathbf{S}^k \mathbf{A} \mathbf{U}_k + b\, \mathbf{S}^k \mathbf{Q}_k + \mathbf{RHS}_{DG1} \right), \tag{136}$$

$$\mathbf{Q}_{VCJH} \equiv \mathbf{Q}_k = \left(\widetilde{\mathcal{M}}^k\right)^{-1} \left(\mathcal{S}^k \mathbf{U}_k + \mathbf{RHS}_{DG2} \right). \tag{137}$$

Upon comparing $\mathbf{R}_{VCJH}$ in Eq. (136) to $\mathbf{R}_{DG}$ in Eq. (132) and $\mathbf{Q}_{VCJH}$ in Eq. (137) to $\mathbf{Q}_{DG}$ in Eq. (133), one observes that the mass matrices of the VCJH scheme and the unfiltered, collocation-based, nodal DG scheme appear to be different. However, if $\mathbf{R}_{DG}$ is multiplied by the invertible filter matrix $\mathbf{F}_1$ and $\mathbf{Q}_{DG}$ is multiplied by the invertible filter matrix $\mathbf{F}_2$, one obtains the following filtered, collocation-based, nodal DG approach

$$\mathbf{F}_1\, \mathbf{R}_{DG} = \mathbf{F}_1 \left(\mathbf{M}^k\right)^{-1} \left(-\mathbf{S}^k \mathbf{A} \mathbf{U}_k + b\, \mathbf{S}^k \mathbf{Q}_k + \mathbf{RHS}_{DG1} \right), \tag{138}$$

$$\mathbf{F}_2\, \mathbf{Q}_{DG} = \mathbf{F}_2 \left(\mathcal{M}^k\right)^{-1} \left(\mathcal{S}^k \mathbf{U}_k + \mathbf{RHS}_{DG2} \right), \tag{139}$$

which is identical to the VCJH approach in Eqs. (136) and (137) provided that the following equations hold

$$\mathbf{F}_1 \left(\mathbf{M}^k\right)^{-1} = \left(\widetilde{\mathbf{M}}^k\right)^{-1} = \left(\mathbf{M}^k + \mathbf{K}^k\right)^{-1}, \tag{140}$$

$$\mathbf{F}_2 \left(\mathcal{M}^k\right)^{-1} = \left(\widetilde{\mathcal{M}}^k\right)^{-1} = \left(\mathcal{M}^k + \mathcal{K}^k\right)^{-1}, \tag{141}$$

or (equivalently) the filters take the following form

$$\mathbf{F}_1 = \left(\mathbf{I} + \left(\mathbf{M}^k\right)^{-1} \mathbf{K}^k\right)^{-1}, \qquad \mathbf{F}_2 = \left(\mathcal{I} + \left(\mathcal{M}^k\right)^{-1} \mathcal{K}^k\right)^{-1}, \tag{142}$$

where $\mathcal{I}$ is the identity matrix in $\mathbb{R}^{3Np \times 3Np}$. Note that the filters $\mathbf{F}_1$ and $\mathbf{F}_2$ exist and are invertible as long as $\mathbf{K}^k$ and $\mathcal{K}^k$ are symmetric, positive-semidefinite matrices, which is guaranteed to be the case for all VCJH schemes (for $c \geq 0$ and $\kappa \geq 0$). If $c \neq 0$ or $\kappa \neq 0$, then $\mathbf{K}^k$ or $\mathcal{K}^k$ contains nontrivial entries, and one recovers a filtered DG approach. Conversely, if $c = 0$ and $\kappa = 0$, then $\mathbf{K}^k$ and $\mathcal{K}^k$ vanish, and one recovers the unfiltered DG approach.

The process of forming filters $\mathbf{F}_1$ and $\mathbf{F}_2$ is described in detail in "Appendix B". The general form of the filters is discussed, and it is shown that the filters act on the highest order polynomial modes (p^{th} degree modes) of the orthonormal basis function expansions of the residual $\mathbf{R}_{DG}$ and the auxiliary variable $\mathbf{Q}_{DG}$. In the next sections, numerical experiments will show that these filters are effective in damping spurious oscillations in the highest order polynomial modes, leading to larger explicit time-step limits for certain VCJH schemes.

In summary, it has been shown that the VCJH schemes for linear advection–diffusion problems on tetrahedra are equivalent to a class of collocation-based, nodal DG schemes that impose filters $\mathbf{F}_1$ and $\mathbf{F}_2$ (Eq. (142)) on the residual $\mathbf{R}_{DG}$ and the auxiliary variable $\mathbf{Q}_{DG}$. As the VCJH approach (from sections 2 - 4) and the filtered DG approach (from this section) are mathematically identical, the reader can implement whichever approach is more convenient for their particular application and software architecture. In particular, one may easily implement the proposed filtering approach within an existing DG implementation. This enables one to employ the VCJH schemes without having to construct the associated correction fields ($\phi_{f,l}$ and $\psi_{f,l}$).

6 Maximizing the Explicit Time-Step Limits of the VCJH Schemes for Linear Advection Problems

The parameters c and κ have an effect on the explicit time-step limit and the accuracy of a VCJH scheme. Williams et al. [38] have shown that choosing $\kappa = c$ and $0 \leq c \leq c_+$ yields stable and accurate results for linear advection–diffusion problems on triangles, where c_+ is a value of c that maximizes the explicit time-step limit for linear advection problems. Values of $c > c_+$ were still found to be stable, but resulted in a reduction in the explicit time-step limits and the orders of accuracy of the schemes. In light of these results, it was desirable to determine values of c_+ for linear advection problems on tetrahedra. In response, Williams [37] employed classical von Neumann analysis (as outlined in [10,21,26,32]) in order to determine the value of $c = c_+$ that maximizes the explicit time-step limit of the VCJH schemes for a 3D, canonical, linear advection problem. For the sake of completeness, the values of c_+ (determined in [37]) for different polynomial orders and different time-stepping

Table 1 Values of c_+ for the 3-stage, 3rd order Runge Kutta scheme (RK33), the 4-stage, 4th order RK scheme (RK44), and a 5-stage, 4th order RK scheme (RK54) [8]

	$p = 2$	$p = 3$	$p = 4$	$p = 5$
RK33	2.22e−02	6.53e−04	1.18e−05	1.25e−07
RK44	2.99e−02	7.33e−04	1.23e−05	1.31e−07
RK54	3.07e−02	5.45e−04	9.92e−06	1.10e−07

schemes are summarized in Table 1. Several of these values are utilized in the numerical experiments of the following section.

7 Numerical Experiments on the Linear Advection–Diffusion Equation

In an effort to further evaluate the performance of the VCJH schemes, they were employed to solve a model linear advection–diffusion problem, and their orders of accuracy and explicit time-step limits were computed.

The governing equation for the model linear advection–diffusion problem took the following form

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{a}u) = b\, \Delta u, \tag{143}$$

where the wave velocity vector $\mathbf{a}$ and the diffusion coefficient b were given the following values: $\mathbf{a} = \left(a_x, a_y, a_z\right) = \left(1/2, 1/2, \sqrt{2}/2\right)$ and $b = 0.01$. Approximate solutions to Eq. (143) were sought within the domain $\mathbf{\Omega} = [-1, 1] \times [-1, 1] \times [-1, 1]$, with periodic boundary conditions imposed. At time $t = 0$, the solution was initialized to $u = \sin(\pi x) \sin(\pi y) \sin(\pi z)$ throughout $\mathbf{\Omega}$, and thereafter, the solution was marched forward in time from $t = 0$ to $t = 1$ using an explicit 5 stage, 4th order, Runge–Kutta time-stepping scheme (RK54) due to Carpenter and Kennedy [8]. At each time-step, the advective numerical fluxes were computed using the Lax–Friedrichs approach with $\lambda = 1$ and the common solutions and diffusive numerical fluxes were computed using the LDG approach with $\tau = 1$ and $\beta = \pm 0.5\mathbf{n}_-$.

The numerical experiments (described above) were used to evaluate the accuracy and stability properties of two 'representative' VCJH schemes: the collocation-based nodal DG scheme with $c = 0$ and $\kappa = 0$, and the scheme with $c = c_+$ and $\kappa = \kappa_+ = c_+$. The orders of accuracy and explicit time-step limits of these two VCJH schemes were computed as follows:

1. The orders of accuracy were computed for $p = 2$ to $p = 5$ on a sequence of regular tetrahedral grids. These grids were obtained by dividing the domain $\mathbf{\Omega}$ into $\tilde{N}^3$ cubic elements of equal size, and then dividing each of these elements into 6 tetrahedral elements of equal size, resulting in grids with a total of $N = 6\tilde{N}^3$ tetrahedral elements. Grids with $\tilde{N} = 4, 6, 8, 12, 16, 24, 32, 48,$ and 64 were created, and on these grids, the accuracy of the approximate solution was evaluated at $t = 1$ using the L2 norm of the error between the approximate solution and the exact solution, where the exact solution took the following form

$$u_{exact} = \exp\left(-3\, b\, \pi^2 t\right) \sin\left(\pi\, (x - a_x t)\right) \sin\left(\pi\, \left(y - a_y t\right)\right) \sin\left(\pi\, (z - a_z t)\right).$$

   The approximate solution was expected to converge towards the exact solution at a rate of h^{p+1}, where h was the mesh spacing.
   In a similar fashion, the accuracy of the solution gradient was evaluated at $t = 1$ using the L2 norm of the error between the approximate solution gradient and the exact solution

Table 2 Accuracy of VCJH schemes for the advection–diffusion problem with $\mathbf{a} = \left(1/2, 1/2, \sqrt{2}/2\right)$ and $b = 0.01$ on the grids with $\tilde{N} = 4$ to $\tilde{N} = 64$

		c_{dg}, κ_{dg}				c_+, κ_+			
p	$\tilde{N}$	L_2 u error	$O(L_2)$	L_2 ∇u error	$O(L_2)$	L_2 u error	$O(L_2)$	L_2 ∇u error	$O(L_2)$
2	4	6.29e−02		1.16e+00		2.96e−01		2.47e+00	
	6	1.84e−02	3.04	5.46e−01	1.86	9.95e−02	2.69	1.31e+00	1.58
	8	7.92e−03	2.92	3.07e−01	2.00	4.18e−02	3.02	8.06e−01	1.68
	12	2.40e−03	2.94	1.31e−01	2.10	1.19e−02	3.10	3.88e−01	1.80
	16	1.00e−03	3.03	6.97e−02	2.20	4.79e−03	3.16	2.21e−01	1.97
	24	2.87e−04	3.09	2.83e−02	2.22	1.27e−03	3.27	9.01e−02	2.21
	32	1.18e−04	3.10	1.50e−02	2.20	4.78e−04	3.40	4.44e−02	2.46
	48	3.36e−05	3.09	6.27e−03	2.16	1.16e−04	3.50	1.53e−02	2.63
	64	1.39e−05	3.07	3.41e−03	2.11	4.20e−05	3.53	7.02e−03	2.70
3	4	1.72e−02		3.75e−01		5.97e−02		1.11e+00	
	6	3.18e−03	4.16	1.07e−01	3.09	1.55e−02	3.33	4.23e−01	2.37
	8	9.24e−04	4.30	4.20e−02	3.25	5.21e−03	3.78	1.85e−01	2.87
	12	1.70e−04	4.18	1.13e−02	3.24	1.02e−03	4.02	5.24e−02	3.12
	16	5.22e−05	4.10	4.50e−03	3.21	3.10e−04	4.15	2.04e−02	3.28
	24	1.01e−05	4.06	1.24e−03	3.18	5.54e−05	4.25	5.11e−03	3.41
	32	3.14e−06	4.04	5.02e−04	3.14	1.59e−05	4.34	1.85e−03	3.54
	48	6.13e−07	4.03	1.43e−04	3.11	2.66e−06	4.41	4.20e−04	3.65
	64	1.93e−07	4.02	5.88e−05	3.08	7.40e−07	4.45	1.45e−04	3.71
4	4	2.59e−03		8.00e−02		1.76e−02		3.84e−01	
	6	3.55e−04	4.90	1.48e−02	4.17	2.99e−03	4.36	9.62e−02	3.42
	8	8.65e−05	4.91	4.49e−03	4.14	7.91e−04	4.63	3.37e−02	3.64
	12	1.15e−05	4.98	8.33e−04	4.15	1.15e−04	4.76	7.11e−03	3.84
	16	2.70e−06	5.03	2.52e−04	4.15	2.82e−05	4.88	2.23e−03	4.03
	24	3.49e−07	5.05	4.73e−05	4.13	3.72e−06	5.00	4.04e−04	4.22
5	4	4.69e−04		1.51e−02		3.53e−03		1.01e−01	
	6	4.31e−05	5.88	1.91e−03	5.10	4.45e−04	5.11	1.72e−02	4.37
	8	7.56e−06	6.05	4.30e−04	5.19	9.48e−05	5.38	4.65e−03	4.56
	12	6.44e−07	6.08	5.28e−05	5.17	9.78e−06	5.60	6.84e−04	4.73
	16	1.12e−07	6.06	1.22e−05	5.10	1.87e−06	5.75	1.68e−04	4.89
	24	9.68e−09	6.05	2.07e−06	4.37	1.74e−07	5.85	2.17e−05	5.04

The advective numerical flux was computed using a Lax–Friedrichs flux with $\lambda = 1$ and the diffusive numerical flux was computed using a LDG flux with $\tau = 1$ and $\beta = \pm 0.5\mathbf{n}_-$

gradient. In this case, the approximate solution gradient was expected to converge towards the exact solution gradient at a rate of h^p.

Note that, in each of the numerical experiments used to determine the rates of convergence of the solution and its gradient, the time-steps were chosen small enough to avoid effecting the spatial accuracy of the schemes.

Finally, note that due to the high accuracy of the schemes with $p = 4$ and $p = 5$, reasonable results were obtained by computing the error on the coarser meshes with $\tilde{N} = 4, 6, 8, 12, 16$, and 24 while neglecting the finest meshes with $\tilde{N} = 32, 48$, and 64.

Table 3 Time-step limits of VCJH schemes for the advection–diffusion problem with $\mathbf{a} = \left(1/2, 1/2, \sqrt{2}/2\right)$ and $b = 0.01$ on the grids with $\tilde{N} = 24$ and 64

p	$\tilde{N}$	c_{dg}, κ_{dg} $\Delta t'_{lim}$	c_+, κ_+ $\Delta t'_{lim}$
2	64	3.24e−04	6.66e−04
3	64	1.51e−04	2.45e−04
4	24	4.72e−04	6.94e−04
5	24	2.74e−04	3.76e−04

The advective numerical flux was computed using a Lax–Friedrichs flux with $\lambda = 1$ and the diffusive numerical flux was computed using a LDG flux with $\tau = 1$ and $\beta = \pm 0.5\mathbf{n}_-$

2. The explicit time-step limits were computed for $p = 2$ and $p = 3$ on the grid with $\tilde{N} = 64$, and for $p = 4$ and $p = 5$ on the grid with $\tilde{N} = 24$. In each case, the maximum time-step limit was taken to be the maximum time-step for which the solution remained bounded at $t = 1000\,\Delta t$ (i.e. boundedness was evaluated after the first 1,000 time-steps). Using this criterion, each maximum time-step limit was determined via an iterative process, which computed the maximum time-step to within an estimated tolerance of 1 %.

The orders of accuracy and explicit time-step limits of the VCJH schemes are presented in Tables 2 and 3. Table 2 demonstrates that the expected order of accuracy is obtained by both the scheme with $c = 0$ and $\kappa = 0$ and the scheme with $c = c_+$ and $\kappa = \kappa_+$, for all values of p, except for $p = 5$ for which roundoff errors appear to have effected the results. In addition, note that for $p = 2$ and $p = 3$, the scheme with $c = c_+$ and $\kappa = \kappa_+$ appears to be superconvergent, in some cases achieving more than $1/2$ an order of accuracy above that which was expected. Table 3 demonstrates that the scheme with $c = c_+$ and $\kappa = \kappa_+$ has the larger explicit time-step limits. In particular, for $p = 2$, the scheme with $c = c_+$ and $\kappa = \kappa_+$ has an explicit time-step limit which is 2.06x larger than that of the collocation-based nodal DG scheme (with $c = 0$ and $\kappa = 0$).

8 Conclusion

A new class of energy stable FR schemes has been proposed for tetrahedral elements. These schemes (referred to as VCJH schemes) utilize the VCJH correction functions and fields in order to correct the solution and the flux in the advection–diffusion equation. It has been shown that these schemes are provably stable for linear advection–diffusion problems in 3D, for all orders of accuracy on unstructured grids. Furthermore, it has been shown that the schemes can be parameterized by two constant scalars c and κ, and that for appropriate choices of these scalars, a class of filtered collocation-based nodal DG schemes can be recovered. Finally, numerical experiments have demonstrated that the VCJH schemes are stable and accurate for linear model problems, and that a certain VCJH scheme possesses an explicit time-step limit that is more than 2x greater than that of the collocation-based nodal DG scheme. Based on these results, it appears that the VCJH schemes represent a promising approach for solving advection–diffusion problems on unstructured meshes of tetrahedral elements. A natural extension of this research would be to employ the VCJH schemes to simulate nonlinear advective and diffusive phenomena on unstructured grids, with an emphasis on simulating fluid-flow phenomena that are governed by the Navier–Stokes equations.

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9 Appendix A: Constructing the Energy Stable (VCJH) Correction Fields

In this section, a procedure will be presented for constructing energy stable (VCJH) correction fields $\phi_{f,l}$ and $\psi_{f,l}$ that satisfy Eqs. (43) and (53), respectively.

9.1 Preliminaries

Recall that $\phi_{f,l} \equiv \hat{\nabla} \cdot \mathbf{h}_{f,l}$ and $\psi_{f,l} \equiv \hat{\nabla} \cdot \mathbf{g}_{f,l}$. In accordance with these definitions, it may appear natural to first construct precise expressions for the correction functions $\mathbf{h}_{f,l}$ and $\mathbf{g}_{f,l}$, and thereafter apply the divergence operator $\hat{\nabla}$ to these expressions in order to obtain $\phi_{f,l}$ and $\psi_{f,l}$. However, this is not the best approach, as $\mathbf{h}_{f,l}$ and $\mathbf{g}_{f,l}$ may not be unique. In particular, for $p > 1$ there are an unlimited number of correction functions which have the same divergence (or effectively, the same correction field). In addition, the implementation of the VCJH approach only requires the precise formulation of the correction fields $\phi_{f,l}$ and $\psi_{f,l}$, and not of the correction functions themselves. Specifically, the VCJH approach only requires definitions of the normal components of the correction functions ($\mathbf{h}_{f,l} \cdot \hat{\mathbf{n}}$ and $\mathbf{g}_{f,l} \cdot \hat{\mathbf{n}}$) which are given by Eqs. (23) and (24). In what follows, it will be shown that Eqs. (23), (24), (43), and (53) are sufficient for constructing precise definitions of $\phi_{f,l}$ and $\psi_{f,l}$.

9.2 Constructing the Correction Fields $\phi_{f,l}$

One may arrive at a procedure for constructing the correction fields $\phi_{f,l}$ by manipulating Eq. (43) and utilizing the definition of $\mathbf{h}_{f,l} \cdot \hat{\mathbf{n}}$ (Eqs. (23) and (24)). Recall from section 3, Lemma 3.1, that the correction functions $\mathbf{h}_{f,l}$ and correction fields $\phi_{f,l}$ are required to satisfy Eq. (43), which can be expanded as follows

$$
\begin{aligned}
&\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\, \hat{D}^{(p,v,w)}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^{C}\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right)\\
&\quad=\int_{\boldsymbol{\Gamma}_S}\left(\hat{\mathbf{f}}^{C}\cdot\hat{\mathbf{n}}\right)\hat{\ell}_j\, d\boldsymbol{\Gamma}_S-\int_{\boldsymbol{\Omega}_S}\left(\hat{\nabla}\cdot\hat{\mathbf{f}}^{C}\right)\hat{\ell}_j\, d\boldsymbol{\Omega}_S\\
&\quad=\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\, \hat{D}^{(p,v,w)}\left(\sum_{f=1}^{N_{fe}}\sum_{l=1}^{N_{fp}}\left[\left(\hat{\mathbf{f}}^{\star}_{f,l}-\hat{\mathbf{f}}^{D}_{f,l}\right)\cdot\hat{\mathbf{n}}_{f,l}\right]\phi_{f,l}\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right)\\
&\quad=\int_{\boldsymbol{\Gamma}_S}\left(\sum_{f=1}^{N_{fe}}\sum_{l=1}^{N_{fp}}\left[\left(\hat{\mathbf{f}}^{\star}_{f,l}-\hat{\mathbf{f}}^{D}_{f,l}\right)\cdot\hat{\mathbf{n}}_{f,l}\right]\mathbf{h}_{f,l}\cdot\hat{\mathbf{n}}\right)\hat{\ell}_j\, d\boldsymbol{\Gamma}_S\\
&\qquad-\int_{\boldsymbol{\Omega}_S}\left(\sum_{f=1}^{N_{fe}}\sum_{l=1}^{N_{fp}}\left[\left(\hat{\mathbf{f}}^{\star}_{f,l}-\hat{\mathbf{f}}^{D}_{f,l}\right)\cdot\hat{\mathbf{n}}_{f,l}\right]\phi_{f,l}\right)\hat{\ell}_j\, d\boldsymbol{\Omega}_S. \qquad (144)
\end{aligned}
$$

Upon rearranging and simplifying Eq. (144), one obtains the following

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\, \hat{D}^{(p,v,w)}\left(\phi_{f,l}\right)\hat{D}^{(p,v,w)}\left(\hat{\ell}_j\right) = \int\limits_{\boldsymbol{\Gamma}_S}\left(\mathbf{h}_{f,l}\cdot\hat{\mathbf{n}}\right)\hat{\ell}_j\, d\boldsymbol{\Gamma}_S - \int\limits_{\boldsymbol{\Omega}_S}\left(\phi_{f,l}\right)\hat{\ell}_j\, d\boldsymbol{\Omega}_S. \tag{145}$$

Here, each basis function $\hat{\ell}_j$ is equal to the product of J_k and ℓ_j, each normal component of a correction function $(\mathbf{h}_{f,l}\cdot\hat{\mathbf{n}})$ is defined by Eq. (23) (with $\mathbf{h}_{f,l}$ in place of $\mathbf{g}_{f,l}$), and each correction field $\phi_{f,l}$ remains to be determined. In order to begin the process of computing $\phi_{f,l}$, note that it is a degree p polynomial function which can be expressed as follows

$$\phi_{f,l} = \sum_{\jmath=1}^{N_p}\sigma_\jmath\, L_\jmath\left(\hat{\mathbf{x}}\right), \tag{146}$$

where each $\sigma_\jmath$ is a constant coefficient (yet to be computed) and each basis function $L_\jmath\left(\hat{\mathbf{x}}\right)$ is a member of an orthonormal basis of degree p on the reference element $\boldsymbol{\Omega}_S$ defined as follows

$$L_\jmath\left(\hat{\mathbf{x}}\right) = \sqrt{8}P_u\left(\hat{a}\right)P_v^{(2u+1,0)}\left(\hat{b}\right)\left(1-\hat{b}\right)^u P_w^{(2u+2v+2,0)}\left(\hat{c}\right)\left(1-\hat{c}\right)^{u+v}, \tag{147}$$

$$\jmath = 1 + \frac{\left(11+12p+3p^2\right)u}{6} + \frac{(2p+3)\,v}{2} + w - \frac{(2+p)\,u^2}{2} - uv - \frac{v^2}{2} + \frac{u^3}{6},$$

$$0\le u,\quad 0\le v,\quad 0\le w,\qquad u+v+w\le p,$$

where $P_n^{(\alpha,\beta)}$ is the normalized n^{th} order Jacobi polynomial (as defined in [19]), and where

$$\hat{a} = -2\frac{(1+\hat{x})}{\hat{y}+\hat{z}} - 1,\qquad \hat{b} = 2\frac{(1+\hat{y})}{1-\hat{z}} - 1,\qquad \hat{c} = \hat{z}. \tag{148}$$

In addition, note that each function $\hat{\ell}_j$ in Eq. (145) is a degree p polynomial which can be expressed as follows

$$\hat{\ell}_j = \sum_{\imath=1}^{N_p}\gamma_\imath\, L_\imath\left(\hat{\mathbf{x}}\right), \tag{149}$$

where each constant coefficient $\gamma_\imath$ is a known quantity because each function $\hat{\ell}_j$ is a known quantity.

On substituting Eqs. (146) and (149) into Eq. (145), one obtains

$$\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\,\hat{D}^{(p,v,w)}\left(\sum_{\jmath=1}^{N_p}\sigma_\jmath\, L_\jmath\right)\hat{D}^{(p,v,w)}\left(\sum_{\imath=1}^{N_p}\gamma_\imath\, L_\imath\right)$$
$$= \int\limits_{\boldsymbol{\Gamma}_S}\left(\mathbf{h}_{f,l}\cdot\hat{\mathbf{n}}\right)\left(\sum_{\imath=1}^{N_p}\gamma_\imath\, L_\imath\right)d\boldsymbol{\Gamma}_S - \int\limits_{\boldsymbol{\Omega}_S}\left(\sum_{\jmath=1}^{N_p}\sigma_\jmath\, L_\jmath\right)\left(\sum_{\imath=1}^{N_p}\gamma_\imath\, L_\imath\right)d\boldsymbol{\Omega}_S, \tag{150}$$

or equivalently

$$\sum_{\jmath=1}^{N_p} \sigma_\jmath \sum_{v=1}^{p+1} \sum_{w=1}^{v} c_{vw}\, \hat{D}^{(p,v,w)}\left(L_\jmath\right) \hat{D}^{(p,v,w)}\left(L_\imath\right)$$

$$= \int_{\boldsymbol{\Gamma}_S} \left(\mathbf{h}_{f,l} \cdot \hat{\mathbf{n}}\right) L_\imath \, d\boldsymbol{\Gamma}_S - \sum_{\jmath=1}^{N_p} \sigma_\jmath \int_{\boldsymbol{\Omega}_S} L_\jmath \, L_\imath \, d\boldsymbol{\Omega}_S. \tag{151}$$

Upon noting that $L_\imath$ and $L_\jmath$ are orthonormal polynomials, one may derive the following expression from Eq. (151)

$$\sum_{\jmath=1}^{N_p} \sigma_\jmath \sum_{v=1}^{p+1} \sum_{w=1}^{v} c_{vw}\, \hat{D}^{(p,v,w)}\left(L_\jmath\right) \hat{D}^{(p,v,w)}\left(L_\imath\right) = -\sigma_\imath + \int_{\boldsymbol{\Gamma}_S} \left(\mathbf{h}_{f,l} \cdot \hat{\mathbf{n}}\right) L_\imath \, d\boldsymbol{\Gamma}_S. \tag{152}$$

Equation (152) holds for $\imath = 1, \ldots, N_p$ and provides a system of N_p equations for the N_p unknown coefficients $\sigma_\jmath$. Together, Eqs. (152) and (146) completely define $\phi_{f,l}$.

9.3 Constructing the Correction Fields $\psi_{f,l}$

In following the approach of the previous section, one may arrive at a procedure for constructing the correction fields $\psi_{f,l}$ by manipulating Eq. (53) and utilizing the definition of $\mathbf{g}_{f,l} \cdot \hat{\mathbf{n}}$ (Eqs. (23) and (24)). Once these manipulations (which are omitted for the sake of brevity) are performed, one obtains the following formula for each field $\psi_{f,l}$

$$\psi_{f,l} = \sum_{\jmath=1}^{N_p} \xi_\jmath \, L_\jmath \left(\hat{\mathbf{x}}\right), \tag{153}$$

where the N_p unknown coefficients $\xi_\jmath$ can be obtained from the following system of $\imath = 1, \ldots, N_p$ equations

$$\sum_{\jmath=1}^{N_p} \xi_\jmath \sum_{v=1}^{p+1} \sum_{w=1}^{v} \kappa_{vw}\, \hat{D}^{(p,v,w)}\left(L_\jmath\right) \hat{D}^{(p,v,w)}\left(L_\imath\right) = -\xi_\imath + \int_{\boldsymbol{\Gamma}_S} \left(\mathbf{g}_{f,l} \cdot \hat{\mathbf{n}}\right) L_\imath \, d\boldsymbol{\Gamma}_S. \tag{154}$$

10 Appendix B: Energy Stable (VCJH) Filter Matrices

This section discusses the procedure for forming the energy stable (VCJH) filter matrices and examines the resulting structure of the filter matrices.

10.1 Procedure for Forming the Filter Matrices

The filters $\mathbf{F}_1$ and $\mathbf{F}_2$ are obtained from the matrices $\mathbf{M}^k$, $\mathcal{M}^k$, $\mathbf{K}^k$, and $\mathcal{K}^k$ via Eq. (142). The mass matrices $\mathbf{M}^k$ and $\mathcal{M}^k$ can be constructed from inner products of the nodal basis functions $\ell_j\left(\hat{\mathbf{x}}\right)$ in accordance with Eq. (70). However, it is often difficult to compute the nodal basis functions $\ell_j\left(\hat{\mathbf{x}}\right)$ directly, and one is often better served by using the orthonormal basis functions $L_j\left(\hat{\mathbf{x}}\right)$ in their place. In particular, one may use the orthonormal basis functions to define a 'Vandermonde matrix' $\mathbf{V}^k$ which has the following entries

$$[\mathbf{V}^k]_{ij} = L_j\left(\hat{\mathbf{x}}_i\right), \tag{155}$$

and next, one may use $\mathbf{V}^k$ to compute the mass matrices as follows

$$\mathbf{M}^k = J_k \left(\mathbf{V}^k \left(\mathbf{V}^k \right)^T \right)^{-1}, \tag{156}$$

$$\mathcal{M}^k = J_k \begin{bmatrix} \left(\mathbf{V}^k \left(\mathbf{V}^k \right)^T \right)^{-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(\mathbf{V}^k \left(\mathbf{V}^k \right)^T \right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \left(\mathbf{V}^k \left(\mathbf{V}^k \right)^T \right)^{-1} \end{bmatrix}. \tag{157}$$

Note that the derivation of Eqs. (156) and (157) is discussed in detail in [19].

In a similar fashion, one may construct expressions for $\mathbf{K}^k$ and $\mathcal{K}^k$ in terms of the orthonormal basis functions. Recall that Eqs. (76) and (77) provide expressions for $\mathbf{K}^k$ and $\mathcal{K}^k$ in terms of the matrices $\left(\hat{\mathbf{D}}^{(p,v,w)} \right)^T \hat{\mathbf{D}}^{(p,v,w)}$, where each $\hat{\mathbf{D}}^{(p,v,w)}$ is a matrix which has the following entries

$$[\hat{\mathbf{D}}^{(p,v,w)}]_{ij} = \hat{D}^{(p,v,w)} \left(\ell_j \left(\hat{\mathbf{x}} \right) \right) \Big|_{\hat{\mathbf{x}}_i}. \tag{158}$$

One may use the orthonormal basis functions $L_j \left(\hat{\mathbf{x}} \right)$ to construct similar matrices $\hat{\hat{\mathbf{D}}}^{(p,v,w)}$ which have the following entries

$$[\hat{\hat{\mathbf{D}}}^{(p,v,w)}]_{ij} = \hat{D}^{(p,v,w)} \left(L_j \left(\hat{\mathbf{x}} \right) \right) \Big|_{\hat{\mathbf{x}}_i}. \tag{159}$$

One may then relate each $\hat{\hat{\mathbf{D}}}^{(p,v,w)}$ to each $\hat{\mathbf{D}}^{(p,v,w)}$ by using the following identity

$$\hat{\mathbf{D}}^{(p,v,w)} = \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k \right)^{-1}. \tag{160}$$

Note that the derivation of Eq. (160) is discussed in detail in [19].

Upon substituting Eq. (160) into Eqs. (76) and (77), one obtains the following expressions for $\mathbf{K}^k$ and $\mathcal{K}^k$

$$\mathbf{K}^k = \frac{J_k}{N_p} \sum_{v=1}^{p+1} \sum_{w=1}^{v} c_{vw} \left(\mathbf{V}^k \right)^{-T} \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)} \right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k \right)^{-1}, \tag{161}$$

$$\mathcal{K}^k = \frac{J_k}{N_p} \sum_{v=1}^{p+1} \sum_{w=1}^{v} \kappa_{vw} \begin{bmatrix} \left(\mathbf{V}^k \right)^{-T} \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)} \right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k \right)^{-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(\mathbf{V}^k \right)^{-T} \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)} \right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k \right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \left(\mathbf{V}^k \right)^{-T} \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)} \right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k \right)^{-1} \end{bmatrix}. \tag{162}$$

Next, on substituting Eqs. (161), (162), (156), and (157) into Eq. (142), one obtains the following expressions for $\mathbf{F}_1$ and $\mathbf{F}_2$

$$\begin{aligned}\mathbf{F}_1 &= \left(\mathbf{I} + \frac{1}{N_p}\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw}\, \mathbf{V}^k \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k\right)^{-1}\right)^{-1} \\ &= \mathbf{V}^k\, \hat{\hat{\mathbf{F}}}_1 \left(\mathbf{V}^k\right)^{-1},\end{aligned} \tag{163}$$

where

$$\hat{\hat{\mathbf{F}}}_1 = \left(\mathbf{I} + \frac{1}{N_p}\sum_{v=1}^{p+1}\sum_{w=1}^{v} c_{vw} \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^{-1}, \tag{164}$$

and

$$\begin{aligned}\mathbf{F}_2 &= \left(\mathcal{I} + \frac{1}{N_p}\sum_{v=1}^{p+1}\sum_{w=1}^{v} \kappa_{vw} \begin{bmatrix} \mathbf{V}^k \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k\right)^{-1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}^k \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k\right)^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{V}^k \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \left(\mathbf{V}^k\right)^{-1} \end{bmatrix}\right)^{-1} \\ &= \mathcal{V}^k\, \hat{\hat{\mathbf{F}}}_2 \left(\mathcal{V}^k\right)^{-1},\end{aligned} \tag{165}$$

where

$$\hat{\hat{\mathbf{F}}}_2 = \left(\mathcal{I} + \frac{1}{N_p}\sum_{v=1}^{p+1}\sum_{w=1}^{v} \kappa_{vw} \begin{bmatrix} \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \left(\hat{\hat{\mathbf{D}}}^{(p,v,w)}\right)^T \hat{\hat{\mathbf{D}}}^{(p,v,w)} \end{bmatrix}\right)^{-1}, \tag{166}$$

and

$$\mathcal{V}^k = \begin{bmatrix} \mathbf{V}^k & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{V}^k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{V}^k \end{bmatrix}. \tag{167}$$

Note that Eqs. (164) and (166) define new filtering matrices $\hat{\hat{\mathbf{F}}}_1$ and $\hat{\hat{\mathbf{F}}}_2$. These matrices can be viewed as filters which act on the orthonormal basis (in contrast to $\mathbf{F}_1$ and $\mathbf{F}_2$ which can be viewed as filters which act on the nodal basis). Conveniently, the two sets of filters are related via left and right multiplication by the Vandermonde matrix and its inverse (as shown in Eqs. (163) and (165)).

Now, having established a method for constructing $\mathbf{F}_1$ and $\mathbf{F}_2$ using the orthornormal basis (via $\hat{\hat{\mathbf{F}}}_1$ and $\hat{\hat{\mathbf{F}}}_2$), one may obtain insights into the overall effects of the filtering process by examining the sparsity patterns of $\hat{\hat{\mathbf{F}}}_1$ and $\hat{\hat{\mathbf{F}}}_2$.

10.2 Sparsity Patterns of the Filter Matrices

On evaluating Eq. (164), one finds that $\hat{\hat{\mathbf{F}}}_1$ has the following block structure

$$\hat{\hat{\mathbf{F}}}_1 = \begin{bmatrix} \mathbf{I}_1^B & \mathbf{0} \\ \mathbf{0} & \mathbf{F}_1^B \end{bmatrix}, \tag{168}$$

where $\mathbf{I}_1^B \in \mathbb{R}^{N_p^\ell \times N_p^\ell}$ is an identity matrix, $\mathbf{F}_1^B \in \mathbb{R}^{N_p^u \times N_p^u}$ is a dense matrix of filtering coefficients, $N_p^\ell = N_p - N_p^u$ is the number of orthonormal basis functions of degree $\leq (p-1)$, and $N_p^u = \frac{1}{2}(p+1)(p+2)$ is the number of orthonormal basis functions of degree p. The structure of $\hat{\hat{\mathbf{F}}}_1$ ensures that only the degree p orthonormal basis functions are effected by the filtering matrix. All basis functions of degree $\leq (p-1)$ are multiplied by the identity matrix and remain unaffected.

Similarly, on evaluating Eq. (166), one finds that $\hat{\hat{\mathbf{F}}}_2$ has the following structure

$$\hat{\hat{\mathbf{F}}}_2 = \begin{bmatrix} \mathbf{I}_2^B & \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{F}_2^B & \ddots & & & \vdots \\ \vdots & \ddots & \mathbf{I}_2^B & \mathbf{0} & & \vdots \\ \vdots & & \mathbf{0} & \mathbf{F}_2^B & \ddots & \vdots \\ \vdots & & & \ddots & \mathbf{I}_2^B & \mathbf{0} \\ \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} & \mathbf{F}_2^B \end{bmatrix}, \tag{169}$$

where $\mathbf{I}_2^B \in \mathbb{R}^{N_p^\ell \times N_p^\ell}$ is an identity matrix and $\mathbf{F}_2^B \in \mathbb{R}^{N_p^u \times N_p^u}$ is a dense matrix of filtering coefficients. The structure of $\hat{\hat{\mathbf{F}}}_2$ is similar to the structure of $\hat{\hat{\mathbf{F}}}_1$, as the structure of $\hat{\hat{\mathbf{F}}}_2$ also ensures that only the degree p orthonormal basis functions are effected by the filtering matrix.

In summary, the filters $\mathbf{F}_1$ and $\mathbf{F}_2$ are related (via the Vandermonde matrix) to the filters $\hat{\hat{\mathbf{F}}}_1$ and $\hat{\hat{\mathbf{F}}}_2$ which act on the orthonormal basis functions $L_j(\hat{\mathbf{x}})$, and effect only the highest (degree p) modes of the residual and the auxiliary variable, respectively.

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