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The Spectral Difference Scheme as a Quadrature-Free Discontinuous Galerkin Method

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1. Introduction

High-order numerical schemes that are based on locally discontinuous polynomial approximations on standard unstructured meshes are particularly attractive for nonlinear convection-dominated problems in complex geometry. The Discontinuous Galerkin (DG) method [1] is a well-known example. For moderate levels of accuracy, however, higher order schemes are advantageous only if a particular discretization method supports efficient implementation. Local numerical integration required by the DG approach can be considered a drawback in this regard. For nonlinear conservation laws, where integration necessitates explicit evaluation of analytical and numerical flux functions at quadrature points, numerical quadratures are quite irksome, since a generic optimal node placement for a given accuracy is not known for general mesh elements, in particular simplex elements. One often uses integration rules based on (singular) tensor products, which oversample the solution in order to achieve the desired order of accuracy [2].

In this context the Spectral Difference scheme [3, 4, 5] has been proposed as a collocation-based method, using local interpolation of the strong form of the equation, with the aim to achieve superior efficiency by avoiding volume and surface quadratures altogether, while maintaining conservation. The Spectral Difference approach extends tensor-product-based collocation approaches that had previously been formulated for quadrilateral meshes [6] to more general unstructured-grid elements.

Another approach is given by 'quadrature-free' DG schemes [7] that avoid quadratures by a suitable projection of the nonlinear analytical and numerical flux functions in the interior and on the surface of mesh elements, respectively, onto finite-dimensional spaces. As a consequence all integrations involve only analytically known basis functions, which allows exact evaluation. This requires fewer degrees of freedom compared to suboptimal numerical quadrature.

In this paper we demonstrate that in fact the Spectral Difference Scheme for nonlinear hyperbolic conservation laws can be derived from a standard Discontinuous Galerkin ansatz using the quadrature-free approach. A few judiciously chosen modifications in the projection of analytical and numerical flux functions, along with some well-known identities for the fundamental polynomials of Lagrangian interpolation, are crucial in this derivation.

Furthermore, the Spectral Difference Scheme is identified as a particularly efficient scheme among the class of quadrature-free DG schemes. The derivation presented here not only shows the general equivalency between the collocation-based approach derived from the strong form of the equations, and the Galerkin approach based on the weak form, but also elucidates how the coupling between mesh elements using numerical flux functions, proposed 'ad-hoc' in the collocation-based formulation [3, 4, 5], are precisely the conditions that allow the derivation of the scheme as a quadrature-free DG scheme. The close connection with other nodal DG schemes [8, 9, 10] becomes obvious, while the key difference is in the projection of nonlinear flux functions.

The paper is organized as follows: We briefly and rather informally recall the definition of the Spectral Difference scheme in the classical derivation from the strong form of the governing equations in section 2. Subsequently we demonstrate in section 3 the essential steps for the derivation from the weak form using a DG approach for a nonlinear one-dimensional conservation law. It remains to incorporate the more complicated metric structure in the multi-dimensional case, which is considered in section 4.

2. The Spectral Difference Scheme

Consider the scalar hyperbolic conservation law

$$\frac{\partial u}{\partial t} + \nabla \cdot f(u) = 0, \quad (1)$$

on some domain $\Omega \subset \mathbb{R}^d$, subject to suitable initial and boundary conditions, where $f(u) = (f^{(1)}(u), \dots, f^{(d)}(u))^T$ is a smooth nonlinear flux function. Consider a triangulation $\mathcal{T}_h = \{T_i\}$, such that $\bar{\Omega}_h = \bigcup \bar{T}_i$. By default we consider simplex elements, while occasionally pointing out obvious extensions to other element types. Assume that there exist mappings $\Phi_i : \hat{T} \rightarrow T_i$ with nonsingular Jacobian $J_i = \partial x / \partial \xi$, such that each element in the triangulation can be mapped to a reference domain \hat{T} . Traditionally the Spectral Difference scheme has been derived from the strong form of the governing equations via a projection of the form

$$J_M \left(\frac{\partial u}{\partial t} + \nabla \cdot (I_N f(u)) \right) = 0, \quad (2)$$

where J_M and I_N are interpolation operators defined on the reference domain. The degrees of freedom M and N depend on the local topology, and whether multivariate or tensor-product-based interpolation is used. For simplices one may let I_N be given by multivariate interpolation using polynomials of degree $m + 1$, while for quadrilateral or hexahedral elements one may use tensor products of one-dimensional interpolation. In any case, let $N = N_{m+1}$. Assuming straight sided elements, i.e. $|J_i| = \text{const.}$, the divergence is written in coordinates local to the reference domain

$$\nabla^x \cdot f = \nabla^\xi \cdot \tilde{f}. \quad (3)$$

where $\tilde{f} = J^{-1} f$. Applying the divergence to the projection $(I_N \tilde{f})$ leads to polynomials of order m . Hence, choosing the interpolation J_M , to be exact for such polynomials, i.e. $M = N_m$, the divergence is evaluated exactly at the corresponding nodes. This leads to the scheme

$$\frac{du_{i,j}}{dt} + \sum_{k=1}^{N_{m+1}} (\nabla^\xi \hat{L}_k) \Big|_{\xi_j} \cdot \tilde{f}_k = 0, \quad \forall T_i \in \mathcal{T}_h, \quad j = 1, \dots, N_m, \quad (4)$$

where $u_{i,j}$ is the nodal value at ξ_j , which belongs to the set of interpolation nodes of J_M , and $\hat{L}_j(\xi)$ are the fundamental polynomials of Lagrangian interpolation corresponding to I_N . Coupling between mesh elements is introduced in an ad-hoc manner in the interpolation of the flux function by evaluating the degrees of freedom as

$$\tilde{f}_k = \begin{cases} J^{-1} f(u_{i,k}) & , \quad \hat{\xi}_k \in \hat{T} \\ \tilde{f}^{num} & , \quad \hat{\xi}_k \in \partial \hat{T} \end{cases}, \quad (5)$$

where $\hat{\xi}_k$ belongs to the set of interpolation nodes corresponding to I_N . The coefficients \tilde{f}^{num} are chosen such that $\tilde{f}^{num} \cdot n^\xi = \tilde{h}$, where n^ξ is the outward pointing normal on $\partial \hat{T}$, and \tilde{h} is a standard numerical flux function. Note that this is equivalent to requiring $f^{num} \cdot n = h$ in untransformed space.

The scheme (4) with condition (5) is the Spectral Difference Scheme in semi-discrete form, which may be treated with a suitable time integration scheme. The "ad-hoc" nature of (5) is summarized by the following remarks:

Remark 1. While it is clear that some of the interpolation nodes of the flux function have to reside on the boundary of the elements, it is not clear if there are further requirements as regards the number of nodes on the boundary, or their placement.

Remark 2. Note that the condition $\tilde{f}^{num} \cdot n^\xi = \tilde{h}$ does not uniquely define the local coefficient \tilde{f}_k , as only the normal flux is specified.

Remark 3. For points that are shared by more than one (d-1)-dimensional face, e.g. vertices in 2D, or edges and vertices in 3D, condition (5) is not well-defined. As an additional constraint one often requires that (5) be satisfied for all faces that share the node. For simplices this never leads to an overspecified problem, since at most d faces of dimension (d-1) meet anywhere on ∂T .

The derivation from a Discontinuous Galerkin approach helps clarify these points.

3. Derivation from a Galerkin Ansatz: The One-Dimensional Case

Here we follow to some extent the approach used by Hesthaven et al. [8, 9, 10] to define and analyze nodal Discontinuous Galerkin schemes, while pointing out key steps that are particular to the Spectral Difference scheme. Consider the scalar one-dimensional hyperbolic conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \quad (6)$$

where $f(u)$ is a smooth nonlinear flux function. For the following analysis boundary conditions are immaterial, so we assume either periodic boundary conditions or a pure initial-value problem, with respectively suitable initial conditions. Consider a partition of the real line into subintervals $I_i = (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$ with midpoints $x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$ and volumes $\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$. Without loss of generality we may assume constant cell volumes. Consider the finite-dimensional space \mathcal{V}_h^m of bounded functions v for which $v|_{I_i} \in \mathcal{P}^m(I_i)$, where \mathcal{P}^m is the space of polynomials of maximum degree m . The DG approach is to find $u_h \in \mathcal{V}_h^m$, such that for each cell i

$$\int_{I_i} (u_h)_i \phi \, dx - \int_{I_i} f(u_h) \phi' \, dx + h_{i+\frac{1}{2}} \phi|_{x_{i+\frac{1}{2}}} - h_{i-\frac{1}{2}} \phi|_{x_{i-\frac{1}{2}}} = 0, \quad \forall \phi \in \mathcal{P}^m(I_i), \quad (7)$$

where $h_{i+\frac{1}{2}}$ is a numerical flux function consistent with $f(u)$ at $x_{i+\frac{1}{2}}$, which one usually chooses in the class of Lipschitz-continuous monotone flux functions [1] for easy incorporation of standard TVD stability theory [11].

It is convenient to formulate a Discontinuous Galerkin discretization of (6) in local coordinates, defined by a linear map $\Phi : \mathcal{I} = (1, 1) \rightarrow I_i$ with $\Phi(\xi) = x_i + \xi \frac{1}{2} \Delta x$. Let $\mathcal{S}_m = \{\xi_k; k = 0, \dots, m\}$ be any nodal set allowing unique Lagrangian interpolation on \mathcal{I} . The corresponding fundamental polynomials $l_k(\xi)$, $k = 0, \dots, m$ satisfying $l_k(\xi_j) = \delta_{kj}$ for all $\xi_j \in \mathcal{S}_m$ form a basis for \mathcal{P}^m . Define a projection onto this space using polynomial interpolation

$$u_h|_{I_i} := \sum_{k=0}^m u_{i,k} l_k(\xi), \quad (8)$$

where $u_k = u(\xi_k)$. (We often omit the cell index i whenever reference to a particular cell is clear.) The Discontinuous Galerkin scheme (7) may be written for each cell

$$\frac{\Delta x}{2} \sum_{k=0}^m \dot{u}_k \int_{-1}^1 l_j l_k \, d\xi - \int_{-1}^1 f(u_h) l_j' \, d\xi + h_{i+\frac{1}{2}} l_j(1) - h_{i-\frac{1}{2}} l_j(-1) = 0, \quad j = 0, \dots, m. \quad (9)$$

Consider the quadrature-free DG method, as introduced by Atkins and Shu [7], which has the defining characteristic that the nonlinear flux $f(u_h)$ is projected onto a finite-dimensional space using polynomials of degree $m+1$. Such quadrature-free nodal DG schemes have been extensively reviewed in [10]. Here we use an alternate nodal set $\mathcal{Q}_{m+1} = \{\hat{\xi}_k; k = 0, \dots, m+1\}$ with corresponding fundamental polynomials \hat{l}_k . We impose the additional restriction that the end points $|\xi| = 1$ be included in the set, and we may suppose that $\hat{\xi}_0 = -1$, and $\hat{\xi}_m = 1$. An approximation for the flux function is thus written

$$f_h|_{I_i} := \sum_{k=0}^{m+1} f_{i,k} \hat{l}_k(\xi), \quad (10)$$

where the degrees of freedom f_k are chosen such that

$$f_k = \begin{cases} h_{i-\frac{1}{2}} & , & k = 0 \\ f(u_h(\xi_k)) & , & 0 < k < m+1 \\ h_{i+\frac{1}{2}} & , & k = m+1 \end{cases} . \quad (11)$$

Substituting (10) into eq. (9), and integrating by parts, leads to

$$\frac{\Delta x}{2} \sum_{k=0}^m \dot{u}_k \int_{-1}^1 l_j l_k \, d\xi + \sum_{k=0}^{m+1} f_k \int_{-1}^1 l_j \hat{l}_k' \, d\xi = 0, \quad j = 0, \dots, m. \quad (12)$$

Note that the boundary terms vanish. Define a local solution vector for the degrees of freedom in each cell by $u_i = (u_{i,0}, \dots, u_{i,m})^T$, and likewise a vector $f_i = (f_{i,0}, \dots, f_{i,m+1})^T$ for the flux coefficients (11). The scheme becomes

$$M\dot{u}_i + S f_i = 0, \quad \forall i, \quad (13)$$

where the matrices $M \in \mathbb{R}^{m \times m}$ and $S \in \mathbb{R}^{m \times m+1}$ are defined

$$m_{jk} = \int_{-1}^1 l_k l_j dx, \quad (14)$$

$$s_{jk} = \frac{2}{\Delta x} \int_{-1}^1 l'_k l_j dx. \quad (15)$$

Note that M is positive definite [12], and thus has an inverse, which may be used to define $D \in \mathbb{R}^{m \times m+1}$ with $D = M^{-1}S$. The entries of D are given by $d_{ij} = (2/\Delta x) \hat{l}'_j|_{\xi_i}$, which is easily verified by direct calculation (cf. [12]):

$$\sum_{k=0}^m m_{jk} d_{kn} = \frac{2}{\Delta x} \int_{-1}^1 l_j \sum_{k=0}^m l_k \hat{l}'_n|_{\xi_k} d\xi = \frac{2}{\Delta x} \int_{-1}^1 l_j \hat{l}'_n d\xi = s_{jn}, \quad (16)$$

where the second equality holds because \hat{l}'_j is by definition a polynomial of degree m , and is hence interpolated exactly on the set \mathcal{S}_m . The matrix D is a standard differentiation matrix, and eq. (13) can be written in terms of the degrees of freedom as

$$\dot{u}_{i,j} + \sum_{k=0}^{m+1} l'_k|_{\xi_j} \tilde{f}_{i,k} = 0, \quad \forall i, \quad j = 0, \dots, m, \quad (17)$$

where $\tilde{f} = (\Phi')^{-1} f = 2/(\Delta x) f$, and the flux coefficients f_k are evaluated as in (11). This by definition is the 1D Spectral Difference Scheme.

4. Derivation from a Galerkin Ansatz: The Multidimensional Case

Consider the scalar hyperbolic conservation law (1) on a triangulated domain Ω_h , with each mesh element mapped to a reference domain, as discussed in section 2. We restrict ourselves to straight-sided simplex elements. Anticipating the Discontinuous Galerkin discretization of eq. (1), we integrate by parts against smooth test functions v over a mesh element:

$$\int_{\hat{T}} \frac{\partial u}{\partial t} v |J| d\xi + \int_{\hat{T}} \nabla^\xi \cdot (J^{-1} f) v d\xi = 0, \quad (18)$$

$$\Leftrightarrow \int_{\hat{T}} \frac{\partial u}{\partial t} v d\xi - \int_{\hat{T}} \nabla^\xi v \cdot (J^{-1} f) d\xi + \int_{\partial \hat{T}} v (J^{-1} f) \cdot n^\xi ds = 0, \quad (19)$$

where the cell index i has been omitted, and n^ξ is the outward pointing normal on $\partial \hat{T}$. Consider the finite-dimensional space $\mathcal{V}_h^m = \{v \in L^2(\Omega_h) : v|_{T_i} \circ \Phi_i \in \mathcal{P}^m(\hat{T})\}$, where $\mathcal{P}^m(\hat{T}) = \text{span}\{\xi^\alpha : \xi \in \hat{T}, \alpha_i \geq 0, |\alpha| \leq m\}$, and $\alpha \in \mathbb{N}^d$ is a multiindex. The dimension of the space \mathcal{P}^m is given by

$$N_m^d = \frac{\prod_{k=1}^d (m+k)}{d!}. \quad (20)$$

In the following we often suppress the superscript d . As a particular basis for $\mathcal{P}^m(\hat{T})$ consider the fundamental polynomials L_j of multivariate Lagrangian interpolation, corresponding to a nodal set $\mathcal{S}_m = \{\xi_j, j = 1, \dots, N_m^d\}$, i.e.

$$u_h|_{T_i} := \sum_{j=1}^{N_m} u_{i,j} L_j(\xi), \quad (21)$$

where $u_j = u(\xi_j)$. This leads to the DG discretization

$$\sum_{j=1}^{N_m} \dot{u}_j \int_{\hat{T}} L_j L_k d\xi - \int_{\hat{T}} \nabla^\xi L_k \cdot (J^{-1} f(u_h)) d\xi + \int_{\partial \hat{T}} \tilde{h} L_k ds = 0, \quad k = 1, \dots, N_m, \quad (22)$$

where the numerical flux function \tilde{h} , consistent at any $\xi \in \partial \hat{T}$ with the normal flux $(J^{-1} f) \cdot n^\xi$, has been introduced.

In the multidimensional case the quadrature-free DG approximation necessitates a projection of both the flux function and the numerical flux onto a finite-dimensional space using polynomials of maximum total degree $m + 1$. Here we use multivariate interpolation on a nodal set $\mathcal{Q}_{m+1} = \{\hat{\xi}_j, j = 1, \dots, N_{m+1}^d\}$ with \hat{L}_j the corresponding fundamental polynomials. This leads to

$$\tilde{f}_h := \sum_{j=1}^{N_{m+1}} \tilde{f}_j \hat{L}_j(\xi), \quad (23)$$

where the $\tilde{f}_j = J^{-1}(f_j^{(1)}, \dots, f_j^{(d)})^T$ are vector-valued coefficients to be determined shortly. Substituting this into equation (22) and integrating by parts leads to

$$\sum_{j=1}^{N_m} \dot{u}_j \int_{\hat{T}} L_j L_k d\xi + \sum_{j=1}^{N_{m+1}} \tilde{f}_j \cdot \int_{\hat{T}} L_k \nabla^\xi \hat{L}_j d\xi + \int_{\partial \hat{T}} (\tilde{h} - \tilde{f}_h \cdot n^\xi) \hat{L}_k ds = 0. \quad (24)$$

It remains to produce a projection of the numerical flux \tilde{h} . We may use a (d-1)-dimensional parametrization ζ of each face $e \in \partial \hat{T}$, and make the following assumption:

Assumption 1. The restriction of the d-dimensional nodal set \mathcal{Q}_{m+1} to each face $e \in \partial \hat{T}$ supports a unique (d-1)-dimensional interpolation of order $m + 1$ with corresponding Lagrangian fundamental polynomials $l_k(\zeta)$, where $\zeta \in \partial \hat{T} \subset \mathbb{R}^{d-1}$. We assume that a subset of exactly N_{m+1}^{d-1} points is located on each $e \in \partial \hat{T}$.

Examples of nodes satisfy Assumption 1 are abundant for the triangle [13, 14, 15, 16] and the tetrahedron [9, 17]. Identify the subset $\{\hat{\xi}_{j(k)}, k = 1, \dots, N_{m+1}^{d-1}\} \subset \mathcal{Q}_{m+1}$ located on face $e \in \partial \hat{T}$. The uniqueness of Lagrangian interpolation (cf. [8]) ensures that, for some function g

$$\sum_{j=1}^{N_{m+1}^d} g(\hat{\xi}_j) L_j(\hat{\xi}^e) = \sum_{k=1}^{N_{m+1}^{d-1}} g(\hat{\xi}_{j(k)}) l_k(\zeta), \quad (25)$$

where ξ^e is the restriction of the d-dimensional coordinate ξ on the face e . A consequence of this fact is that if $(J^{-1} f_h) \cdot n^\xi = \tilde{h}$ at the interpolation nodes $\hat{\xi}_{j(k)}$, the surface integral in (24) identically vanishes. This is actually accomplished if the approximation (23) is carried out using eq. (5) that had been introduced in section 2 for the Spectral Difference Scheme.

Define a local vector $u_i = (u_{i,1}, \dots, u_{i,N_m})^T$, and do likewise for the flux coefficients. Upon defining the matrices M with $m_{ij} = \int L_j, L_j d\xi$ and $S^{(l)}$ with $s_{ij}^{(l)} = \int L_i \frac{\partial \hat{L}_j}{\partial \xi_i} d\xi$, the scheme may be written

$$M \dot{u}_i + \sum_{l=1}^d S^{(l)} \tilde{f}^{(l)} = 0, \quad i = 1, \dots, N_{elem}, \quad (26)$$

where N_{elem} is the number of mesh elements, and $\tilde{f}^{(l)} = (\tilde{f}_1^{(l)}, \dots, \tilde{f}_{N_m}^{(l)})^T$, are the coefficients of the flux in l direction, evaluated as in (5). Again following [8], we note that the local mass matrix M is symmetric positive definite, and thus may be inverted. Furthermore, as in the one-dimensional case, there holds $M^{-1} S^{(l)} = D^{(l)}$, where the entries of $D^{(l)}$ are given by $d_{ij}^{(l)} = \frac{\partial \hat{L}_j}{\partial \xi_i} \Big|_{\xi_i}$, which can be verified by noting that $\hat{L}_j(\xi)$ is a polynomial of degree $m + 1$, and hence

$$(MD^{(l)})_{ij} = \sum_{k=1}^{N_m} \int_{\hat{T}} L_i L_k \frac{\partial \hat{L}_j}{\partial \xi_i} \Big|_{\xi_k} d\xi = \int_{\hat{T}} L_i \frac{\partial \hat{L}_j}{\partial \xi_i} d\xi = s_{ij}^{(l)}. \quad (27)$$

Using this identity the scheme can be written in terms of the local degrees of freedom, i.e.

$$\frac{du_{i,j}}{dt} + \sum_{k=1}^{N_{m+1}} (\nabla^{\xi} \hat{L}_k)|_{\xi_j} \cdot \tilde{f}_k = 0. \quad (28)$$

This recovers the Spectral Difference scheme (4).

It is interesting to note that both the underdetermined coupling conditions for the flux function (see remark 2) and the additional constraint identified in remark 3 turn out to be precisely the minimal conditions needed to eliminate the surface integral in the DG derivation pursued here, leading to a particularly efficient version of a quadrature-free DG scheme. Note that we have an additional constraint regarding the placement of nodes on the boundary of elements, stated by Assumption 1. The derivation from the strong form of the equations does not include this constraint, and may thus be viewed as more general, but in turn lacks identification of "good" placement of boundary nodes.

In comparison with similar nodal DG schemes [8, 9, 10], the main difference is that the numerical flux is used in the collocation (23) in a particular way, which leads to elimination of the surface integral in eq. (24). Collocating the analytical flux function at all nodes retains the surface integral, which may be multiplied with a penalty term, simplifying stability analysis [8, 9]. A more thorough investigation into the similarities and differences of these approaches should prove interesting. This is left for future publication.

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