Edge Functions for Spectral Element Methods

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Chapter 1
EDGE FUNCTIONS FOR SPECTRAL ELEMENT METHODS

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Abstract It is common practice in finite element methods to expand the unknowns in nodal functions. The discretization of the gradient, curl and divergence operators requires H^1, (curl) and $H(\mathrm{div})$ function spaces and their discrete representation. Especially in mixed formulations this involved quite some mathematical machinery which can be avoided once we recognize that not all unknowns are associated with point-values. In this short paper higher order basis functions will be presented which have the property that conservation laws become independent of the basis functions. The basis functions proposed in this paper yield a discrete representation of **grad**, **curl** and **div** which are exact and completely determined by the topology of the grid. The discretization of these vector operators is invariant under general bijective transformations.

1.1 Introduction

Mimetic discretization schemes aim to preserve symmetries of the physical system to be modeled. If we are able to represent such symmetries in a discrete setting, we satisfy the associated conservation law in the discrete sense.

Mimetic discretizations are based on the strong analogy between differential geometry and algebraic topology. The global, metric-free description can be rephrased without error in terms of cochains, while the local description requires differential field reconstructions. For an introduction to the interplay between differential forms and cochains the reader is referred to [1, 2, 3, 5, 6, 11, 14].

A key ingredient in mimetic methods is to re-establish the explicit connection between physical variables and the geometric objects these variables are associated with. The operation that connects the physical variable with its associated geometric

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object is *integration*, where the geometry, $\mathscr{C}$, enters the integral as the domain of integration and the physical variable, Φ, appears as the integrand.

$$\int_{\mathscr{C}} \Phi \, dC = \langle \mathscr{C}, \Phi \rangle \in \mathbb{R} \,. \tag{1.1}$$

Equation (1.1) expresses the fact that geometric integration is in fact duality pairing between geometry, $\mathscr{C}$, and physical variables, Φ, since integration is a bilinear operation.

In [8, 9, 12] this approach is applied to spectral element methods. The main ingredient in this approach is the use of spectral basis functions which are associated with points, lines, surfaces and volumes. This paper focuses on the construction of the basis function associated with line segments, the so-called *edge functions*. Since we will consider quadrilateral elements only and employ tensor products to form the spectral element basis, the higher-dimensional basis functions are formed naturally by applying tensor products. For instance, the surface element is the tensor product of two edge functions and one nodal function, whereas the volume basis function is the tensor product of three edge functions.

The outline of the paper is as follows: In Section 1.2 the so-called *edge functions* will be derived for a simple one-dimensional equations. In Section 1.3 the edge functions will be used to discretize the differential operators, **grad**, **curl** and **div**. Concluding remarks can be found in Section 1.4.

1.2 The edge functions

Consider the one-dimensional equation

$$u(\xi) = \frac{d\phi}{d\xi} \,, \quad \xi \in [a,b] \,. \tag{1.2}$$

Let $a = \xi_0 < \xi_1 < \cdots < \xi_{N-1} < \xi_N = b$ be a partitioning of the interval $[a,b]$, then the function $\phi(\xi)$ can be expanded in nodal basis functions

$$\phi(\xi) = \sum_{i=0}^{N} \phi_i h_i(\xi) \,, \tag{1.3}$$

in which $h_i(\xi)$ are Lagrange basis functions through the points ξ_i, $i = 0, \dots, N$ and $\phi_i = \phi(\xi_i)$. The traditional way to discretize (1.2) is to expand $u(\xi)$ in the *same* Lagrangian basis functions $h_i(\xi)$, i.e.

$$u(\xi) = \sum_{i=0}^{N} u_i h_i(\xi) \,. \tag{1.4}$$

If we insert the expansions (1.3) and (1.4) in (1.2) we obtain

$$\sum_{i=0}^{N} u_i h_i(\xi) = \sum_{i=0}^{N} \phi_i \frac{dh_i}{d\xi} \; . \tag{1.5}$$

There are however a few objections to this approach: Firstly, a polynomial of degree N on the left hand side is equated to a polynomial of degree $N-1$ on the right hand side. Secondly, this formulation is *not* invariant under general bijective coordinate transformations. These shortcomings can be attributed to the fact that *u cannot be associated with nodes*. In terms of differential geometry: If ϕ is a 0-form, then $u = d\phi$ is a 1-form which is associated with line segments. On a more engineering level we have that

$$\phi(p) = \phi(q) + \int_p^q u(x)\, dx \; , \tag{1.6}$$

i.e. the point-wise evaluation of ϕ in two arbitrary points p and q is associated with the integral of u over the interval (p,q). Let us therefore define the integral quantities

$$\overline{u}_i = \int_{\xi_{i-1}}^{\xi_i} u(x)\, dx \; , \quad i = 1, \ldots, N \; . \tag{1.7}$$

Note that by defining $\overline{u}_i$ as an integral quantity instead of the value in particular points, we exactly satisfy $\overline{u}_i = \phi_i - \phi_{i-1}$, which is the discrete analogue of the integral relation (1.6). Interpolation of integral quantities is called *histopolation*, see Robidoux, [13].

We have that

$$\begin{aligned}
u^N(\xi) &= \sum_{i=0}^{N} \phi_i dh_i(\xi) \\
&= \sum_{i=0}^{N} (\phi_i - \phi_k)\, dh_i(\xi) \\
&= \sum_{i=0}^{N} \left[- \sum_{j=i+1}^{k} \overline{u}_j + \sum_{j=k+1}^{i} \overline{u}_j \right] dh_i(\xi) \\
&= - \sum_{i=0}^{k-1} dh_i(\xi) \sum_{j=i+1}^{k} \overline{u}_j + \sum_{i=k+1}^{N} dh_i(\xi) \sum_{j=k+1}^{i} \overline{u}_j \\
&= - \sum_{j=1}^{k} \left(\sum_{i=0}^{j-1} dh_i(\xi) \right) \overline{u}_j + \sum_{j=k+1}^{N} \left(\sum_{i=j}^{N} dh_j(\xi) \right) \overline{u}_j
\end{aligned} \tag{1.8}$$

The first line states that the discrete approximation (histopolation) of u, denoted by $u^N(\xi)$, can be exactly expressed as the derivative of the discrete interpolation of $\phi(\xi)$. In the second line we use

$$\sum_{i=0}^{N} h_i(\xi) \equiv 1 \quad \Longrightarrow \quad \sum_{i=0}^{N} dh_i(\xi) = d \sum_{i=0}^{N} h_i(\xi) \equiv 0 \; , \tag{1.9}$$

and in the third line we used $\overline{u}_i = \phi_i - \phi_{i-1}$ repeatedly. In the remaining lines we re-arrange the summations. Since (1.8) is true for all $k = 0, \ldots, N$, we can eliminate k by averaging over all k

$$\begin{aligned}
u^N(\xi) &= \frac{1}{N+1} \sum_{k=0}^{N} u^N(\xi) \\
&= -\frac{1}{N+1} \sum_{k=0}^{N} \sum_{j=1}^{k} \left(\sum_{i=0}^{j-1} dh_i(\xi) \right) \overline{u}_j + \frac{1}{N+1} \sum_{k=0}^{N} \sum_{j=k+1}^{N} \left(\sum_{i=j}^{N} dh_j(\xi) \right) \overline{u}_j \\
&= \frac{1}{N+1} \sum_{j=1}^{N} \left[-(N+1-j)\overline{u}_j \sum_{i=0}^{j-1} dh_i(\xi) + j\overline{u}_j \sum_{i=j}^{N} dh_i(\xi) \right] \\
&= \frac{1}{N+1} \sum_{j=1}^{N} \left[-(N+1)\overline{u}_j \sum_{i=0}^{j-1} dh_i(\xi) + j\overline{u}_j \sum_{i=0}^{N} dh_i(\xi) \right] \\
&= -\sum_{j=1}^{N} \overline{u}_j \sum_{i=0}^{j-1} dh_i(\xi) \,. \qquad (1.10)
\end{aligned}$$

If we now define the basis functions

$$e_j(\xi) = -\sum_{i=0}^{j-1} dh_i(\xi)\,, \quad j = 1, \ldots, N\,, \qquad (1.11)$$

we can express u in terms of the integral quantities $\overline{u}_i$ as

$$u^N(\xi) = \sum_{i=1}^{N} \overline{u}_i e_i(\xi)\,. \qquad (1.12)$$

The basis functions $e_i(\xi)$ can be interpreted as polynomial indicator functions, Figure 1.1, because they satisfy

$$\int_{\xi_{k-1}}^{\xi_k} e_i(x) = \delta_{i,k} = \begin{cases} 1 & \text{if } i = k \\ \\ 0 & \text{if } i \neq k \end{cases} \,. \qquad (1.13)$$

Compare this with the nodal interpolation where we have that $h_i(\xi_j) = \delta_{i,j}$. The basis functions $e_i(\xi)$ correspond to higher order Whitney forms, see [3, 6, 18]. Note that we have $de_j(\xi) = -d \circ d \sum h_i(\xi) \equiv 0$, see for instance Flanders, [7]. This property will be used repeatedly in the next section. If we insert the expansion of u in terms of edge functions into our one-dimensional model problem, we obtain

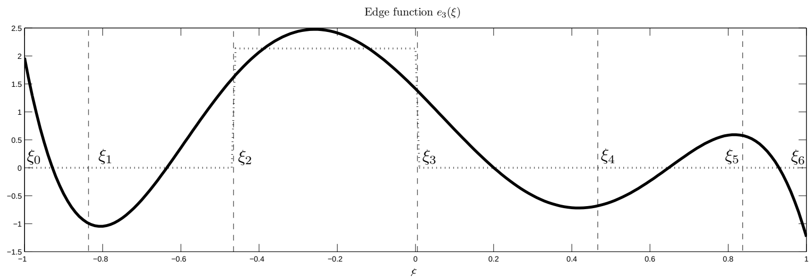

Fig. 1.1 Example of an edge function: Partitioning of the interval [-1,1] with Gauss-Lobatto nodes and the edge function $e_3(\xi)$

$$\begin{aligned}\sum_{i=1}^{N} \bar{u}_i e_i(\xi) &= \sum_{i=0}^{N} \phi_i dh_i(\xi) \\ &= -\sum_{i=1}^{N} (\phi_i - \phi_{i-1}) \sum_{j=0}^{i-1} dh_j(\xi) \\ &= \sum_{i=1}^{N} (\phi_i - \phi_{i-1}) e_i(\xi) \end{aligned} \tag{1.14}$$

This shows that there is strict equality: The polynomial degrees on both sides are the same and this relation remains valid under arbitrary bijective transformations, since the basis functions on both sides of the equality sign transform in the same way. Because the basis functions $e_i(\xi)$ are linearly independent, we in fact have

$$\sum_{i=1}^{N} [\bar{u}_i - (\phi_i - \phi_{i-1})] e_i(\xi) = 0 \quad \Longrightarrow \quad \bar{u}_i - (\phi_i - \phi_{i-1}) = 0 \; . \tag{1.15}$$

This is a purely topological, metric-free relation because all the metric properties are encoded in the basis functions and its form is solely determined by the topology of the grid. Once we know which nodes form the boundary of a given line segment, we can set up this relation. The definitions of $\bar{u}_i$, (1.7), and ϕ_i show that (1.15) is *exact*; no approximations are involved.

The metric-free form, (1.15), resembles a finite volume discretization, see for instance [10, 15, 16, 17] of the sample problem. In the next section discrete representations of vector operators in terms of the edge functions will be addressed. The resulting discrete equations also resemble finite volume discretizations.

1.3 Application of edge functions to grad, curl and div

The gradient operator

$$\text{Consider} \quad u = \mathbf{grad}\,\phi \; . \tag{1.16}$$

Let ϕ be expanded as a tensor product of nodal functions in the coordinates (ξ,η,ζ)

$$\phi(\xi,\eta,\zeta) = \sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N} \phi_{i,j,k} h_i(\xi) h_j(\eta) h_k(\zeta) \; , \tag{1.17}$$

then it can be shown by straightforward calculation that

$$\overline{u}^{\xi}_{i,j,k} = \phi_{i,j,k} - \phi_{i-1,j,k} \; , \quad \overline{u}^{\eta}_{i,j,k} = \phi_{i,j,k} - \phi_{i,j-1,k} \quad \text{and}$$

$$\overline{u}^{\zeta}_{i,j,k} = \phi_{i,j,k} - \phi_{i,j,k-1} \; , \tag{1.18}$$

with

$$u^{\xi}(\xi,\eta,\zeta) = \sum_{i=1}^{N}\sum_{j=0}^{N}\sum_{k=0}^{N} \overline{u}^{\xi}_{i,j,k} e_i(\xi) h_j(\eta) h_k(\zeta) \; ,$$

$$u^{\eta}(\xi,\eta,\zeta) = \sum_{i=0}^{N}\sum_{j=1}^{N}\sum_{k=0}^{N} \overline{u}^{\eta}_{i,j,k} h_i(\xi) e_j(\eta) h_k(\zeta) \; ,$$

$$u^{\zeta}(\xi,\eta,\zeta) = \sum_{i=0}^{N}\sum_{j=0}^{N}\sum_{k=1}^{N} \overline{u}^{\zeta}_{i,j,k} h_i(\xi) h_j(\eta) e_k(\zeta) \; . \tag{1.19}$$

Again, these relations are exact and coordinate free.

The curl operator

Let u be defined along edges, (1.19), then $\omega = \mathbf{curl}\,u$ is given by

$$\overline{\omega}^{\xi}_{i,j,k} = \overline{u}^{\zeta}_{i,j,k} - \overline{u}^{\zeta}_{i,j-1,k} - \overline{u}^{\eta}_{i,j,k} + \overline{u}^{\eta}_{i,j,k-1} \; ,$$

$$\overline{\omega}^{\eta}_{i,j,k} = \overline{u}^{\xi}_{i,j,k} - \overline{u}^{\xi}_{i,j,k-1} - \overline{u}^{\zeta}_{i,j,k} + \overline{u}^{\zeta}_{i-1,j,k} \; ,$$

$$\overline{\omega}^{\zeta}_{i,j,k} = \overline{u}^{\eta}_{i,j,k} - \overline{u}^{\eta}_{i-1,j,k} - \overline{u}^{\xi}_{i,j,k} + \overline{u}^{\xi}_{i,j-1,k} \; , \tag{1.20}$$

with

$$\omega^{\xi}(\xi,\eta,\zeta) = \sum_{i=0}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} \overline{\omega}^{\xi}_{i,j,k} h_i(\xi) e_j(\eta) e_k(\zeta) \; ,$$

$$\omega^{\eta}(\xi,\eta,\zeta) = \sum_{i=1}^{N}\sum_{j=0}^{N}\sum_{k=1}^{N} \overline{\omega}^{\eta}_{i,j,k} e_i(\xi) h_j(\eta) e_k(\zeta) \; ,$$

$$\omega^{\zeta}(\xi,\eta,\zeta) = \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=0}^{N} \overline{\omega}^{\zeta}_{i,j,k} e_i(\xi) e_j(\eta) h_k(\zeta) \; .$$

If u is a gradient, (1.18), then $\omega^{\xi} = \omega^{\eta} = \omega^{\zeta} \equiv 0$, which implies

$$u = \mathbf{grad}\,\phi \quad \Longleftrightarrow \quad \mathbf{curl}\,u \equiv 0 \; . \tag{1.21}$$

These relations are metric-free and invariant under bijective transformations.

The divergence operator

Consider the divergence equation

$$a = \mathbf{div}\, f \ . \tag{1.22}$$

Given fluxes defined over surfaces. Let the flux vector be expanded as

$$\begin{aligned} f^{\xi}(\xi,\eta,\zeta) &= \sum_{i=0}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} \overline{f}^{\xi}_{i,j,k} h_i(\xi) e_j(\eta) e_k(\zeta) \ , \\ f^{\eta}(\xi,\eta,\zeta) &= \sum_{i=1}^{N}\sum_{j=0}^{N}\sum_{k=1}^{N} \overline{f}^{\eta}_{i,j,k} e_i(\xi) h_j(\eta) e_k(\zeta) \ , \\ f^{\zeta}(\xi,\eta,\zeta) &= \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=0}^{N} \overline{f}^{\zeta}_{i,j,k} e_i(\xi) e_j(\eta) h_k(\zeta) \ . \end{aligned} \tag{1.23}$$

If a is expanded in terms of volume basis functions

$$a(\xi,\eta,\zeta) = \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} \overline{a}_{i,j,k} e_i(\xi) e_j(\eta) e_k(\zeta) \ , \tag{1.24}$$

the divergence equation reduces to

$$\overline{a}_{i,j,k} = \overline{f}^{\xi}_{i,j,k} - \overline{f}^{\xi}_{i-1,j,k} + \overline{f}^{\eta}_{i,j,k} - \overline{f}^{\eta}_{i,j-1,k} + \overline{f}^{\zeta}_{i,j,k} - \overline{f}^{\zeta}_{i,j,k-1} \ . \tag{1.25}$$

Again we see that the divergence equation reduces to a topological equation which is independent of the basis functions. And therefore these relations will remain unchanged under general coordinate transformations. The unknowns $\overline{a}_{i,j,k}$ and $\overline{f}^{\xi}_{i,j,k}$ represent

$$\overline{a}_{i,j,k} = \int_{\xi_{i-1}}^{\xi_i}\int_{\eta_{j-1}}^{\eta_j}\int_{\zeta_{k-1}}^{\zeta_k} a(\xi,\eta,\zeta)\, d\xi d\eta d\zeta \ , \quad \overline{f}^{\xi}_{i,j,k} = \int_{\eta_{j-1}}^{\eta_j}\int_{\zeta_{k-1}}^{\zeta_k} f^{\xi}(\xi,\eta,\zeta)\, d\eta d\zeta \ , \tag{1.26}$$

it follows that (1.25) is an exact representation of the divergence equation. No numerical approximations are involved. If the fluxes f are the curl of a vector ω, i.e., $f = \mathbf{curl}\, \omega$ then also in the discrete setting we have

$$\mathbf{div}\, f = 0 \quad \Longleftrightarrow \quad f = \mathbf{curl}\, \omega \tag{1.27}$$

1.4 Concluding remarks

In this paper the edge functions $e_i(x)$ were derived, representing basis functions along line segments. Using tensor products, these edge functions can be used to represent variables defined over surfaces and volumes. The extension to higher order dimensions is straightforward. Using these basis functions the discrete representation of the gradient, curl and divergence are purely topological and independent of the basis functions. These relations are exact; no numerical approximation is involved. Since these operations are metric-free, they are preserved under bijective mappings and in this sense they extend the Thomas-Raviart and Nédélec elements, which are only invariant under affine transformations. Although an arbitrary partitioning was considered, for spectral element methods usually the Gauss-Lobatto nodes are taken. An application of these edge function for partial differential equations in curvilinear coordinates can be found in Bouman, [4].

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