

Hierarchical Universal Matrices for Sensitivity Analysis by Curvilinear Finite Elements

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Abstract—A new method for calculating the geometric sensitivities of curvilinear finite elements is presented. Approximating the relevant metric tensors by hierarchical orthogonal polynomials enables the sensitivity matrices to be integrated analytically. The resulting numerical method is based on pre-calculated universal matrices and achieves significant savings in computer runtime over conventional techniques based on numerical integration. Moreover, there exists a representation limit for the geometry, i.e., the degree of basis functions fully determines a critical order of the geometry expansion, beyond which the derivatives of the finite-element matrices will remain constant. To validate the suggested approach, a numerical example is presented.

Keywords—curvilinear, eigenvalues, finite elements, hierarchical, sensitivity, universal matrix.

I. INTRODUCTION

Higher-order finite elements (FEs) are attractive because they yield exponential convergence in case of smooth fields. However, to harvest their full potential, curvilinear boundaries must be taken into account. Typically, the resulting metric terms do not admit analytical integration of the FE matrices. Numerical integration is possible, though computationally expensive. An alternative is polynomial interpolation or approximation of the metric terms followed by exact integration. The resulting algorithms [1], [2] achieve significant savings in computer runtime, by utilizing pre-calculated universal matrices (UMs) [3]. Applications such as sensitivity analysis and gradient-based optimization require not only the FE matrices but also their derivatives with respect to the parameters [4], [5]. This paper presents a procedure for computing such derivatives at low computational cost. It employs hierarchical UMs and applies to both straight-sided and curvilinear FEs. The method will be demonstrated by reference to the $\mathbf{H}(\text{curl})$ shape functions of [6].

II. MODEL PROBLEM

Consider a cavity resonator Ω whose boundary Γ_E is a perfect electric conductor (PEC). Maxwell's equations lead to the following eigenvalue problem (EVP) for the modal electric field \mathbf{E} and the corresponding free-space wavenumber k :

$$\nabla \times (\boldsymbol{\mu}_r^{-1} \nabla \times \mathbf{E}) - k^2 \boldsymbol{\varepsilon}_r \mathbf{E} = \mathbf{0} \quad \text{in } \Omega, \quad (1a)$$

$$\hat{\mathbf{n}} \times \mathbf{E} = \mathbf{0} \quad \text{in } \Gamma_E. \quad (1b)$$

Herein $\boldsymbol{\mu}_r$ and $\boldsymbol{\varepsilon}_r$ denote the relative magnetic permeability and electric permittivity, respectively. The weak formulation of the EVP (1) reads:

$$\int_{\Omega} \nabla \times \mathbf{E} \cdot \boldsymbol{\mu}_r^{-1} \nabla \times \mathbf{w} \, dx - k^2 \int_{\Omega} \mathbf{E} \cdot \boldsymbol{\varepsilon}_r \mathbf{w} \, dx = 0 \quad \forall \mathbf{w} \in \mathbf{H}_E(\text{curl}; \Omega, \Gamma_E). \quad (2)$$

FE discretization using a set of $\mathbf{H}(\text{curl})$ basis functions \mathbf{w}_a^m , where $(\cdot)^m$ indicates the polynomial degree, leads to the algebraic EVP:

$$(\mathbf{S} - k^2 \mathbf{T}) \mathbf{v} = \mathbf{0}, \quad (3)$$

with eigenvector \mathbf{v} . Herein the stiffness matrix \mathbf{S} and the mass matrix \mathbf{T} are given by:

$$[\mathbf{S}^{mn}]_{aq} = \int_{\Omega} \nabla \times \mathbf{w}_a^m \cdot \boldsymbol{\mu}_r^{-1} \nabla \times \mathbf{w}_q^n \, dx, \quad (4a)$$

$$[\mathbf{T}^{mn}]_{aq} = \int_{\Omega} \mathbf{w}_a^m \cdot \boldsymbol{\varepsilon}_r \mathbf{w}_q^n \, dx. \quad (4b)$$

Provided that $\boldsymbol{\mu}_r, \boldsymbol{\varepsilon}_r \in \mathbb{R}^+$ and both matrices are real symmetric, \mathbf{S} and \mathbf{T} is positive definite. Let \mathbf{S} and \mathbf{T} depend smoothly on a parameter τ , and let the considered eigenvalue k_i^2 be of multiplicity one. Then, according to [7], the sensitivity of k_i^2 with respect to τ is given by:

$$\frac{\partial}{\partial \tau} k_i^2 = \mathbf{v}_i^T \left(\frac{\partial}{\partial \tau} \mathbf{S} - k_i^2 \frac{\partial}{\partial \tau} \mathbf{T} \right) \mathbf{v}_i, \quad (5)$$

provided that the eigenvectors are normalized according to:

$$\mathbf{v}_i^T \mathbf{T} \mathbf{v}_i = \mathbf{I}. \quad (6)$$

Thus, sensitivity analysis requires the considered eigenpair (k_i^2, \mathbf{v}_i) as well as the matrix derivatives $\frac{\partial}{\partial \tau} \mathbf{S}$ and $\frac{\partial}{\partial \tau} \mathbf{T}$.

III. HIERARCHICAL UNIVERSAL MATRICES

In an unstructured mesh, FEs of different sizes and shapes are present. It is customary to compute the contributions of a single FE Ω_e , i.e., the element matrices \mathbf{S}_e and \mathbf{T}_e , from a reference domain $\hat{\Omega}_e$ equipped with local coordinates $\boldsymbol{\varphi}$. Let $\hat{\mathbf{w}}_a^m(\boldsymbol{\varphi})$ denote the basis functions on $\hat{\Omega}_e$ and $\mathbf{J}(\boldsymbol{\varphi})$ the

Jacobian of the geometry mapping. By means of the metric tensors $\widehat{\Lambda}^1(\varphi)$ and $\widehat{\Lambda}^2(\varphi)$ defined by:

$$\widehat{\Lambda}^1 = |\mathbf{J}| \mathbf{J}^{-T} \boldsymbol{\varepsilon}_r \mathbf{J}^{-1}, \quad (7a)$$

$$\widehat{\Lambda}^2 = |\mathbf{J}|^{-1} \mathbf{J} \boldsymbol{\mu}_r^{-1} \mathbf{J}^T, \quad (7b)$$

the element matrices \mathbf{S}_e and \mathbf{T}_e take the form:

$$[\mathbf{S}_e^{mn}]_{aq} = \int_{\widehat{\Omega}_e} \nabla_\varphi \times \widehat{\mathbf{w}}_a^m \cdot \widehat{\Lambda}^2 \nabla_\varphi \times \widehat{\mathbf{w}}_q^n \, d\varphi, \quad (8a)$$

$$[\mathbf{T}_e^{mn}]_{aq} = \int_{\widehat{\Omega}_e} \widehat{\mathbf{w}}_a^m \cdot \widehat{\Lambda}^1 \widehat{\mathbf{w}}_q^n \, d\varphi. \quad (8b)$$

In [3] a hierarchical basis of scalar polynomials $b_l^k(\varphi)$ which are pairwise orthogonal on $\widehat{\Omega}_e$ was introduced:

$$\int_{\widehat{\Omega}_e} b_l^k(\varphi) b_i^p(\varphi) \, d\varphi = \begin{cases} 1 & \text{for } (k, l) = (p, i), \\ 0 & \text{else.} \end{cases} \quad (9)$$

Here $(\cdot)^k$ gives the polynomial order, and $(\cdot)_l$ denotes functions of same order. Expanding $\widehat{\Lambda}^{(\cdot)}$ in the basis $\{b_l^k\}$ leads to:

$$\widehat{\Lambda}^{(\cdot)}(\varphi) = \sum_{k=0}^{\infty} \sum_{l=1}^{L(k)} \widehat{\Lambda}_{kl}^{(\cdot)} b_l^k(\varphi), \quad \varphi \in \widehat{\Omega}, \quad (10)$$

wherein $\widehat{\Lambda}_{kl}$ stands for a constant matrix-valued coefficient and $L(k)$ for the number of homogeneous polynomials of order k . Thanks to orthonormality (9), the calculation of $\widehat{\Lambda}_{kl}$ reduces to:

$$\widehat{\Lambda}_{kl} = \int_{\widehat{\Omega}} \widehat{\Lambda}(\varphi) b_l^k \, d\varphi. \quad (11)$$

In the general case, the evaluation of (11) requires numerical integration. Note that this is the only source of error in the proposed method.

Eq. (10) yields a polynomial representation for (8), which hereby becomes accessible to analytical integration. We thus have:

$$\mathbf{S}^{mn} = \sum_{k=0}^{m+n-2} \sum_{l=1}^{L(k)} \sum_{i,j} \left[\widehat{\Lambda}_{kl}^2 \right]_{ij} \mathbf{S}_{ijl}^{mnk}, \quad (12a)$$

$$\mathbf{T}^{mn} = \sum_{k=0}^{m+n} \sum_{l=1}^{L(k)} \sum_{i,j} \left[\widehat{\Lambda}_{kl}^1 \right]_{ij} \mathbf{T}_{ijl}^{mnk}, \quad (12b)$$

wherein \mathbf{S}_{ijl}^{mnk} and \mathbf{T}_{ijl}^{mnk} are metric-independent UMs. They are independent of the geometry and need to be computed only once. The UMs inherit the hierarchical structure of the basis functions [6]. Thanks to orthogonality, the results of the truncated sums in (12) are exact; see [3].

IV. UNIVERSAL MATRICES FOR SENSITIVITY ANALYSIS

When the geometry is parameterized by τ , the Jacobian \mathbf{J} and, in consequence, the metric tensors $\boldsymbol{\Lambda}^{(\cdot)}$ become τ depen-

dent, whereas the $\widehat{\mathbf{w}}_a^m(\varphi)$ remain unchanged. In view of (7) and (8), the derivatives of the element matrices read:

$$\frac{\partial}{\partial \tau} [\mathbf{S}_e^{mn}]_{aq} = \int_{\widehat{\Omega}_e} \nabla_\varphi \times \widehat{\mathbf{w}}_a^m \cdot \frac{\partial}{\partial \tau} \widehat{\Lambda}^2 \nabla_\varphi \times \widehat{\mathbf{w}}_q^n \, d\varphi, \quad (13a)$$

$$\frac{\partial}{\partial \tau} [\mathbf{T}_e^{mn}]_{aq} = \int_{\widehat{\Omega}_e} \widehat{\mathbf{w}}_a^m \cdot \frac{\partial}{\partial \tau} \widehat{\Lambda}^1 \widehat{\mathbf{w}}_q^n \, d\varphi. \quad (13b)$$

The structure of (13) implies that $\frac{\partial}{\partial \tau} \mathbf{S}$ and $\frac{\partial}{\partial \tau} \mathbf{T}$ may be constructed from UMs too, by a method similar to Section III: The polynomial expansions of $\frac{\partial}{\partial \tau} \boldsymbol{\Lambda}^{(\cdot)}$ in terms of b_l^k read:

$$\frac{\partial}{\partial \tau} \widehat{\Lambda}^{(\cdot)}(\varphi) = \sum_{k=0}^{\infty} \sum_{l=1}^{L(k)} \frac{\partial}{\partial \tau} \widehat{\Lambda}_{kl}^{(\cdot)} b_l^k(\varphi), \quad \varphi \in \widehat{\Omega}. \quad (14)$$

Substituting the series expansion (14) for the derivatives of the metric tensors in (13) leads to polynomial representations which, again, allow for analytical integration. We arrive at:

$$\frac{\partial}{\partial \tau} \mathbf{S}^{mn} = \sum_{k=0}^{m+n-2} \sum_{l=1}^{L(k)} \sum_{i,j} \left[\frac{\partial}{\partial \tau} \widehat{\Lambda}_{kl}^2 \right]_{ij} \mathbf{S}_{ijl}^{mnk}, \quad (15a)$$

$$\frac{\partial}{\partial \tau} \mathbf{T}^{mn} = \sum_{k=0}^{m+n} \sum_{l=1}^{L(k)} \sum_{i,j} \left[\frac{\partial}{\partial \tau} \widehat{\Lambda}_{kl}^1 \right]_{ij} \mathbf{T}_{ijl}^{mnk}. \quad (15b)$$

Eq. (15) provides an efficient procedure for computing the matrix derivatives, based on the same UMs as (12). It can be shown that metric expansions of order $m+n-2$ and $m+n$ for \mathbf{S} and \mathbf{T} , respectively, yield exact results; see the Appendix for a detailed derivation. Hence, the maximum order of the metric expansion required in the general curvilinear case is:

$$k = 2p - 2 \quad \text{for } \frac{\partial}{\partial \tau} \mathbf{S}, \quad (16a)$$

$$k = 2p \quad \text{for } \frac{\partial}{\partial \tau} \mathbf{T}. \quad (16b)$$

A. Sensitivity with Respect to Geometry Parameters

Let the geometry be described by \mathbf{H}^1 interpolatory FE basis functions $L_i(\varphi)$, using the parameter-dependent locations of the element nodes $\mathbf{r}_i(\tau)$ as interpolation points. By denoting the matrix of node coordinates by $\mathbf{R}(\tau)$ and the vector of basis functions by $\mathbf{L}(\varphi)$, the position vector $\mathbf{x}(\tau)$ takes the form:

$$\mathbf{x}(\tau) = \mathbf{f}(\tau, \varphi) = \sum_i \mathbf{r}_i(\tau) L_i(\varphi) = \mathbf{R}(\tau) \mathbf{L}(\varphi). \quad (17)$$

Thus, the derivative of the Jacobian reads:

$$\frac{\partial}{\partial \tau} \mathbf{J} = \frac{\partial}{\partial \tau} \nabla_\varphi \mathbf{f}^T = [\nabla_\varphi \mathbf{L}^T] \left[\frac{\partial}{\partial \tau} \mathbf{R}^T \right], \quad (18)$$

and the derivatives of the metric tensors $\hat{\mathbf{\Lambda}}^1$ and $\hat{\mathbf{\Lambda}}^2$, which are needed in (13), are obtained by:

$$\begin{aligned} \frac{\partial}{\partial \tau} \hat{\mathbf{\Lambda}}^1 &= \hat{\mathbf{\Lambda}}^1 \operatorname{tr} \left[\mathbf{J}^{-1} \frac{\partial}{\partial \tau} \mathbf{J} \right] - |\mathbf{J}| \left(\mathbf{J}^{-T} \frac{\partial \mathbf{J}^T}{\partial \tau} \mathbf{J}^{-T} \boldsymbol{\varepsilon}_r \mathbf{J}^{-1} \right) \\ &\quad - |\mathbf{J}| \left(\mathbf{J}^{-T} \boldsymbol{\varepsilon}_r \mathbf{J}^{-1} \frac{\partial \mathbf{J}}{\partial \tau} \mathbf{J}^{-1} \right), \end{aligned} \quad (19a)$$

$$\begin{aligned} \frac{\partial}{\partial \tau} \hat{\mathbf{\Lambda}}^2 &= |\mathbf{J}|^{-1} \left(\frac{\partial \mathbf{J}}{\partial \tau} \boldsymbol{\mu}_r^{-1} \mathbf{J}^T + \mathbf{J} \boldsymbol{\mu}_r^{-1} \frac{\partial \mathbf{J}^T}{\partial \tau} \right) \\ &\quad - \hat{\mathbf{\Lambda}}^2 \operatorname{tr} \left[\mathbf{J}^{-1} \frac{\partial}{\partial \tau} \mathbf{J} \right]. \end{aligned} \quad (19b)$$

B. Computational Cost

In the following, $N(p)$ denotes the number of scalar polynomials up to order p and $G(p)$ the number of interpolation points of a quadrature method for the reference tetrahedron which is exact for polynomials up to order p ; see [8].

With the present method, computing the derivatives of the element matrices involves two steps: The first is the k -th order expansion of the metric tensors according to (10) and (11), respectively. This is computationally cheap and will not be further considered.

The second step is the actual calculation of $\frac{\partial}{\partial \tau} \mathbf{S}$ and $\frac{\partial}{\partial \tau} \mathbf{T}$. Since the polynomial expansions for the metric tensors allow (13) to be integrated analytically with the help of UMs, the numbers of scaled matrix additions A_S and A_T are solely determined by the number of metric coefficients $\hat{\mathbf{\Lambda}}_{kl}$ in (10) and (14): Each metric tensor is a symmetric 3×3 matrix, with six independent entries. Hence, the number of coefficients is $6N(k)$, and we have:

$$A_S = 6N(k) \stackrel{(16a)}{=} 6N(2p-2) \quad \text{for } \frac{\partial}{\partial \tau} \mathbf{S}, \quad (20a)$$

$$A_T = 6N(k) \stackrel{(16b)}{=} 6N(2p) \quad \text{for } \frac{\partial}{\partial \tau} \mathbf{T}. \quad (20b)$$

Further optimizations are possible by exploiting the fact that, thanks to the hierarchical structure of the considered FE basis functions, many of the integrals (13) are of lower order.

For comparison, consider methods that compute the element matrices $\frac{\partial}{\partial \tau} \mathbf{S}$ and $\frac{\partial}{\partial \tau} \mathbf{T}$ by numerical integration in the curvilinear case. Eq. (13) implies that the quadrature rule ought to be exact for polynomials of order $2(p-1) + k$ and $2p + k$, respectively. Thus, the resulting numbers of scaled matrix additions, A_S^{num} and A_T^{num} , are:

$$A_S^{num} = 6G(2p+k-2) \stackrel{(16a)}{=} 6G(4p-4), \quad (21a)$$

$$A_T^{num} = 6G(2p+k) \stackrel{(16b)}{=} 6G(4p). \quad (21b)$$

Table I and Table II compare the numerical cost of the UM-based scheme (20) and numerical integration (21), for the $\frac{\partial}{\partial \tau} \mathbf{S}$ and $\frac{\partial}{\partial \tau} \mathbf{T}$ matrix, respectively. The quadrature method of [8] is used. The superiority of the suggested approach is evident.

TABLE I
NUMBER OF SCALED MATRIX ADDITIONS FOR THE STIFFNESS MATRIX

Method	FE Order p	Order of Metric Expansion k						
		0	1	2	3	4	5	6
Num. integ.	1	6	6	24	48	84	84	144
	2	24	48	84	84	144	216	276
	3	84	84	144	216	276	366	486
This work	1	6	6	6	6	6	6	6
	2	6	24	60	60	60	60	60
	3	6	24	60	120	210	210	210

TABLE II
NUMBER OF SCALED MATRIX ADDITIONS FOR THE MASS MATRIX

Method	FE Order p	Order of Metric Expansion k						
		0	1	2	3	4	5	6
Num. integ.	1	24	48	84	84	144	216	276
	2	84	84	144	216	276	366	486
	3	144	216	276	366	486	654	840
This work	1	6	24	60	60	60	60	60
	2	6	24	60	120	210	210	210
	3	6	24	60	120	210	336	504

V. NUMERICAL EXAMPLE

We consider a lossless spherical resonator, with the material properties of free space and a perfect electric conductor on its outer boundary. The radius r of the sphere depends on a parameter τ ,

$$r(\tau) = (1 + \tau)r_0, \quad (22)$$

wherein the nominal radius r_0 is taken to be $r_0 = 1$ m. The goal is to compute the sensitivity of the resonance eigenvalue k^2 of the dominant mode with respect to τ .

To avoid technicalities with the analysis of convergence rates due to eigenvalues of higher multiplicity, only one quarter of the structure is modeled. Thereby, the symmetry planes are taken to be perfect magnetic conductors. The structure is discretized into 512 tetrahedra, using piecewise 3rd order polynomials for the element shapes. The reference values for the numerical studies below have been obtained from analytical calculations [9].

Fig. 1 presents the relative error in the sensitivity of the dominant eigenvalue: High-order FEs yield the optimal rate of convergence only if the curvilinear boundary is approximated well enough, i.e., if the approximation orders of the metric tensors $\hat{\mathbf{\Lambda}}^1$ and $\hat{\mathbf{\Lambda}}^2$ are chosen correctly. It is also interesting to see that approximation by constant metrics ($k = 0$) performs much better than conventional interpolation by straight-sided tetrahedra.

Fig. 2 demonstrates that increasing the metric approximation beyond a FE-order specific limit does not improve the solution, because the FE matrices are sharp already. Beyond this point, the error in the solution is solely due to the approximation properties of the FE basis.

Since the fields are smooth, the rate of convergence of the eigenvalue sensitivity $\frac{\partial}{\partial \tau} k^2$ is expected to be exponential in the mesh parameter h . The rates obtained from the authors' numerical data, for metric expansion order $k = 6$, are of order $\mathcal{O}(h^{2.04p})$ and $\mathcal{O}(h^{2.07p})$ for basis function order $p = 2$ and $p = 3$, respectively.

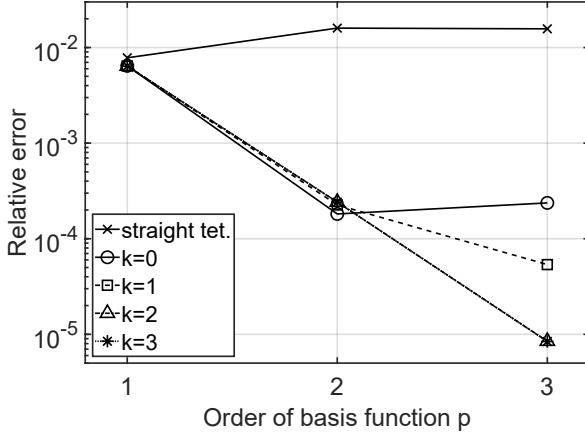


Fig. 1. Relative error in sensitivity of dominant eigenvalue k^2 versus order of FE basis p . Parameter: order of metric approximation k .

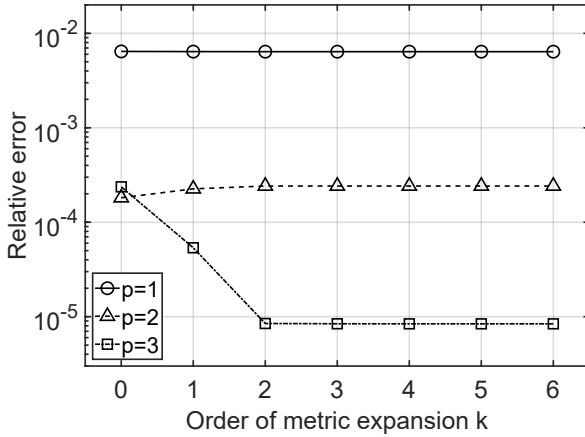


Fig. 2. Relative error in sensitivity of dominant eigenvalue k^2 versus order of metric approximation k . Parameter: order of FE basis p .

VI. CONCLUSIONS

An improved method for computing the sensitivity of FE solutions with respect to geometric parameters has been presented. Its key feature is the use of orthogonal hierarchical polynomial expansions for the metric terms present in the FE matrices. This allows the element matrices and their derivatives to be obtained from precomputed universal matrices, even in the curvilinear case. In consequence, the computational costs of the proposed method are lower than those of traditional methods which use numerical integration. Moreover, it has been shown that there exists a critical order of the metric

expansion, which is determined by the degree of the FE basis functions, beyond which the FE matrices and their derivatives will remain constant.

The validity of the suggested approach has been demonstrated by a numerical example, for the sensitivity of resonance wavenumbers.

VII. APPENDIX

Substituting the hierarchical expansion (14) for the metric tensors in (13) leads to UMs of the form:

$$[\mathbf{S}_{ijl}^{mnk}]_{aq} = \int_{\hat{\Omega}_e} [\nabla_\varphi \times \hat{\mathbf{w}}_a^m]_i b_l^k [\nabla_\varphi \times \hat{\mathbf{w}}_q^n]_j d\varphi, \quad (23a)$$

$$[\mathbf{T}_{ijl}^{mn}]_{aq} = \int_{\hat{\Omega}_e} [\hat{\mathbf{w}}_a^m]_i b_l^k [\hat{\mathbf{w}}_q^n]_j d\varphi. \quad (23b)$$

Let \mathcal{P}^q denote the space of scalar polynomials of order q on $\hat{\Omega}_e$. The products of (the curl of) the basis functions in (23) are readily seen to satisfy:

$$[\nabla_\varphi \times \hat{\mathbf{w}}_a^m]_i [\nabla_\varphi \times \hat{\mathbf{w}}_q^n]_j \in \mathcal{P}^{m+n-2}, \quad (24a)$$

$$[\hat{\mathbf{w}}_a^m]_i [\hat{\mathbf{w}}_q^n]_j \in \mathcal{P}^{m+n}. \quad (24b)$$

Expressing these in the hierarchical basis $\{b_i^p\}$ yields:

$$[\nabla_\varphi \times \hat{\mathbf{w}}_a^m]_i [\nabla_\varphi \times \hat{\mathbf{w}}_q^n]_j = \sum_p^{m+n-2} \sum_i \sigma_i^p b_i^p, \quad (25a)$$

$$[\hat{\mathbf{w}}_a^m]_i [\hat{\mathbf{w}}_q^n]_j = \sum_p^{m+n} \sum_i \tau_i^p b_i^p, \quad (25b)$$

with constant coefficients σ_i^p and τ_i^p . In consequence, the entries of the UMs of (23) take the form:

$$[\mathbf{S}_{ijl}^{mn}]_{aq} = \sum_p^{m+n-2} \sum_i \sigma_i^p \int_{\hat{\Omega}_e} b_i^p b_l^k d\varphi, \quad (26a)$$

$$[\mathbf{T}_{ijl}^{mn}]_{aq} = \sum_p^{m+n} \sum_i \tau_i^p \int_{\hat{\Omega}_e} b_i^p b_l^k d\varphi. \quad (26b)$$

Thanks to orthogonality (9), the integrals in (26a) vanish for $k > m + n - 2$ and those in (26b) for $k > m + n$. This completes the proof of (16).

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