A C^2 Trivariate Macro-Element Based on the Clough-Tocher-Split of a Tetrahedron

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Abstract. A C^2 trivariate macro-element is constructed based on the Clough-Tocher split of a tetrahedron into four subtetrahedra. The element uses supersplines of degree 13, and provides optimal order approximation of smooth functions.

§1. Introduction

Macro-elements are useful for creating local methods for fitting scattered data, and are also an important tool in the numerical solution of partial differential equations. While bivariate macro-elements are well-understood, much less is known in the trivariate case, see Remarks 1–3. Our aim in this paper is to describe and analyze a new C^2 trivariate macro-element.

For our purposes, a trivariate macro-element defined on a tetrahedron T will consist of a pair $(\mathcal{S}, \Lambda)$, where $\mathcal{S}$ is space of splines (piecewise polynomial functions) defined on a partition of T into subtetrahedra, and $\Lambda := \{\lambda_i\}_{i=1}^n$ is a set of linear functionals which define values and derivatives of a spline s at certain points in T in such a way that for any given values z_i, there is a unique spline $s \in \mathcal{S}$ with $\lambda_i s = z_i$ for $i = 1, \ldots, n$. These functionals are called the nodal degrees of freedom of the element.

Suppose now that $\triangle$ is a tetrahedral partition of a polyhedral domain Ω in $\mathbb{R}^3$, i.e, a collection of tetrahedra whose union is Ω with the property that any two tetrahedra in $\triangle$ touch each other only at vertices, along edges, or at common triangular faces. We say that a macro-element has smoothness C^r provided that if the element is used to construct an interpolating spline locally on each tetrahedron of $\triangle$, then the resulting piecewise function is C^r continuous globally. Several C^1 macro-elements have been constructed in the literature, see [1,19,20]. Here we are interested in the C^2 case.

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At present the only known C^2 macro-element seems to be the element of [21], which is based on polynomials of degree 17 and which does not require splitting the tetrahedron T. As is well known from the bivariate case, to get macro-elements using piecewise polynomials of lower degree, one has to split T. Here we will use a split of T into four subtetrahedra about an interior point v_T.

The paper is organized as follows. In Sect. 2 we introduce some notation. The main results of the paper are in Sect. 3, where we describe our C^2 macro-element and derive error bounds for its use in Hermite interpolation of smooth functions. Sect. 4 is devoted to some technical lemmas on polynomial interpolation. We conclude the paper with several remarks in Sect. 5.

§2. Preliminaries

Throughout the paper, we write $\mathcal{P}_d^j$ for the $\binom{d+j}{j}$ dimensional linear space of polynomials of degree d in j variables. Given a tetrahedral partition $\triangle$ of a polyhedral domain Ω, we define

$$\mathcal{S}_d^r(\triangle) := \{s \in C^r(\Omega) : s|_T \in \mathcal{P}_d^3, \text{ for all } T \in \triangle\}.$$

In dealing with polynomials and splines, we will make use of well-known Bernstein–Bézier methods as used for example in [1–4,7–20]. As usual, given a tetrahedron $T := \langle v_1, v_2, v_3, v_4\rangle$ and a polynomial p of degree d, we denote the B-coefficients of p by $c_{ijkl}^{T,d}$ and associate them with the domain points $\xi_{ijkl}^{T,d} := (iv_1 + jv_2 + kv_3 + lv_4)/d$, where $i+j+k+l = d$. We write $\mathcal{D}_{T,d}$ for the set of all domain points associated with T. We say that the domain point $\xi_{ijkl}^{T,d}$ has distance $d-i$ from the vertex v_1, with similar definitions for the other vertices. We say that $\xi_{ijkl}^{T,d}$ is at a distance $i+j$ from the edge $e := \langle v_3, v_4\rangle$, with similar definitions for the other edges of T. If $\triangle$ is a tetrahedral partition of a set Ω, we write $\mathcal{D}_{\triangle,d}$ for the collection of all domain points associated with tetrahedra in $\triangle$, where points on edges and faces are not repeated.

Given $\rho > 0$, we refer to the union $D_\rho(v)$ of all domain points which are within a distance ρ from v as the ball of radius ρ around v. Similarly, we refer to the union $R_\rho(v)$ of all domain points which are at a distance ρ from v as the shell of radius ρ around v. If T is a tetrahedron of $\triangle$, we shall use the short-hand notations $D_\rho^T(v) := D_\rho(v) \cap T$ and $R_\rho^T(v) := R_\rho(v) \cap T$. If e is an edge of $\triangle$, we define the tube of radius ρ around e to be the set of domain points whose distance to e is at most ρ.

If F is a face of a tetrahedron T, then the domain points in $\mathcal{D}_{T,d}$ which lie on F associated with a trivariate polynomial on T can be considered to be the domain points of a bivariate polynomial of degree d defined on the triangle F. If $F := \langle u, v, w\rangle$ is such a face, we write $\mathcal{D}_{d,F} := \{\xi_{ijk}^{F,d} := \frac{iu+jv+kw}{d}\}_{i+j+k=d}$ for this set of domain points.

Given any multi-index $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, we write D^α for the partial derivative $D_x^{\alpha_1} D_y^{\alpha_1} D_z^{\alpha_1}$. For each edge $e := \langle u, v\rangle$ of a tetrahedron $T \in \triangle$, suppose X_e is the plane perpendicular to e at the point u. We endow X_e with Cartesian coordinate axes whose origin lies at the point u. Then for any multi-index $\beta = (\beta_1, \beta_2)$, we define D_e^β to be the corresponding derivative. It corresponds to a directional derivative of order $|\beta| := \beta_1 + \beta_2$ in a direction lying in X_e. Associated with e we also need notation for the following points:

$$\eta_{e,j}^i := \frac{(i-j+1)u + jv}{i+1}, \qquad j = 1, \ldots, i, \tag{2.1}$$

for all $i > 0$. If $F := \langle u, v, w \rangle$ is a face of T, then we write D_F for the unit normal derivative associated with F, pointing into the tetrahedron. Finally, if η is a point in $\mathbb{R}^3$, we write ε_η for the point-evaluation functional associated with η, so that for any trivariate function, $\varepsilon_\eta f := f(\eta)$.

Suppose $\mathcal{S}$ is a linear subspace of $\mathcal{S}_d^0(\triangle)$, and suppose $\mathcal{N}$ is a collection of linear functionals λ, where λs is defined by a combination of values or derivatives of s at a point η_λ in Ω. Then we say that $\mathcal{N}$ is a nodal determining set (NDS) for $\mathcal{S}$ provided that if $s \in \mathcal{S}$ and $\lambda s = 0$ for all $\lambda \in \mathcal{N}$, then $s \equiv 0$. It is called a nodal minimal determining set (NMDS) for $\mathcal{S}$ provided that for each set of real numbers $\{z_\lambda\}_{\lambda \in \mathcal{N}}$, there exists a unique $s \in \mathcal{S}$ such that $\lambda s = z_\lambda$ for all $\lambda \in \mathcal{N}$.

§3. A C^2 Macro-element Based on the Clough-Tocher Split

Given a tetrahedron $T := \langle v_1, v_2, v_3, v_4 \rangle$, let v_T be a point in the interior of T. Then we define the Clough-Tocher split T_{CT} of T to consist of the four subtetrahedra obtained by connecting v_T to each of the vertices of T. We write $\mathcal{V}_T$, $\mathcal{E}_T$, and $\mathcal{F}_T$ for the sets of vertices, edges, and faces of T, respectively. Our C^2 macro-element will be based on the following space of supersplines defined on T_{CT}:

$$\begin{aligned} \mathcal{S}_2(T_{CT}) := \{ & s \in C^2(T) : s|_{\widetilde{T}} \in \mathcal{P}_{13}^3 \text{ all } \widetilde{T} \in T_{CT}, \\ & s \in C^3(e) \text{ for all } e \in \mathcal{E}_T, \\ & s \in C^6(v) \text{ for all } v \in \mathcal{V}_T, \text{ and } s \in C^{12}(v_T)\}. \end{aligned} \tag{3.1}$$

As usual, if v is a vertex of T_{CT}, then $s \in C^\rho(v)$ means that all polynomial pieces of s defined on tetrahedra sharing the vertex v have common derivatives up to order ρ at v. If e is an edge of T_{CT}, then $s \in C^\mu(e)$ means that all subpolynomials of s defined on tetrahedra sharing the edge e have common derivatives up to order μ on e. We have not chosen the supersmoothness in the definition of $\mathcal{S}_2(T_{CT})$ arbitrarily. The C^3 supersmoothness around edges and the C^6 supersmoothness at vertices is required in order to get a macro-element which joins smoothly with neighboring macro-elements, see Remark 4. This forces us to use polynomials of degree 13. We have required the C^{12} supersmoothness at v_T in order to remove unnecessary degrees of freedom from our macro-element.

For each face F of T, let

$$\begin{aligned} A_F^0 &:= \{\xi_{ijk}^{F,13} : i,j,k \geq 4\} = \{\xi_{544}^{F,13}, \xi_{454}^{F,13}, \xi_{445}^{F,13}\}, \\ A_F^1 &:= \{\xi_{ijk}^{F,12} : i,j,k \geq 3\}, \\ A_F^2 &:= \{\xi_{ijk}^{F,11} : i,j,k \geq 2\} \setminus \{\xi_{272}^{F,11}, \xi_{227}^{F,11}, \xi_{722}^{F,11}\}, \end{aligned} \tag{3.2}$$

We emphasize that all of these points are on faces F of T (and not inside the tetrahedron T). We mark the position of these points with $\oplus$ in Fig. 1. Note that the cardinalities of these three sets are 3, 10, and 18, respectively. In addition, let

$$A_T := \{\xi_{ijk}^{T,12} : i,j,k \geq 2\}. \tag{3.3}$$

This set has cardinality 35, and all points are in the interior of T. Using the notation of the previous section, we now have the following theorem.

Theorem 3.1. *The space $\mathcal{S}_2(T_{CT})$ has dimension 615. Moreover,*

$$\mathcal{N} := \bigcup_{v \in \mathcal{V}_T} \mathcal{N}_v \cup \bigcup_{e \in \mathcal{E}_T} \mathcal{N}_e \cup \bigcup_{F \in \mathcal{F}_T} (\mathcal{N}_F^0 \cup \mathcal{N}_F^1 \cup \mathcal{N}_F^2) \cup \mathcal{N}_{v_T} \tag{3.4}$$

is a nodal minimal determining set for $\mathcal{S}_2(T_{CT})$, where

1) $\mathcal{N}_v := \bigcup_{|\alpha| \leq 6} \{\varepsilon_v D^\alpha\}$,
2) $\mathcal{N}_e := \bigcup_{i=1}^{3} \bigcup_{j=1}^{i} \{\varepsilon_{\eta_{e,j}^i} D_e^\alpha\}_{|\alpha|=i}$,
3) $\mathcal{N}_F^0 := \{\varepsilon_\xi\}_{\xi \in A_F^0}$,
4) $\mathcal{N}_F^1 := \{\varepsilon_\xi D_F\}_{\xi \in A_F^1}$,
5) $\mathcal{N}_F^2 := \{\varepsilon_\xi D_F^2\}_{\xi \in A_F^2}$,
6) $\mathcal{N}_{v_T} := \{\varepsilon_\xi\}_{\xi \in \mathcal{A}_T}$.

Proof: To show that $\mathcal{N}$ is a nodal minimal determining set for $\mathcal{S}_2(T_{CT})$, we need to show that setting the values $\{\lambda s\}_{\lambda \in \mathcal{N}}$ of a spline $s \in \mathcal{S}_2(T_{CT})$ uniquely determines all B-coefficients of s. First, for each $v \in \mathcal{V}_T$, the C^6 smoothness at v implies that setting $\{\lambda s\}_{\lambda \in \mathcal{N}_v}$ uniquely determines the B-coefficients corresponding to domain points in $D_6(v)$. Moreover, for each edge $e \in \mathcal{E}_T$, the C^3 smoothness around e implies that setting $\{\lambda s\}_{\lambda \in \mathcal{N}_e}$ uniquely determines the B-coefficients of s in the tubes of radius 3 around e.

We now examine the coefficients corresponding to domain points on the shell $R_{13}(v_T)$, i.e., on the outer faces of T_{CT}. Let $F := \langle v_1, v_2, v_3 \rangle$ be a face of this shell as shown in Fig. 1 (left). We can consider the coefficients of s corresponding to the domain points on F as the coefficients $\{c_\xi^{F,13}\}_{\xi \in \mathcal{D}_{F,13}}$ of the bivariate polynomial $s|_F$ of degree 13. The coefficients corresponding to the domain points marked with black dots and triangles in Fig. 1 (left) are already uniquely determined as they lie either in the 6-disks around the vertices of F, or in the 3-tubes around its edges.

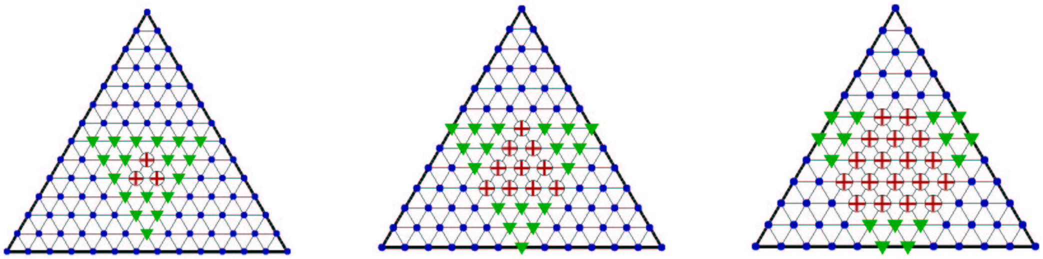

Fig. 1. The point sets $\mathcal{A}_F^0$, $\mathcal{A}_F^1$, and $\mathcal{A}_F^2$.

This leaves 3 coefficients corresponding to the domain points marked with $\oplus$ in Fig. 1 (left). These are precisely the coefficients $\{c_\xi^{F,13}\}_{\xi\in\mathcal{A}_F^0}$, and are determined from the interpolation conditions corresponding to $\mathcal{N}_F^0$. This leads to a 3×3 system with matrix $M_3 := [B_\xi^{F,13}(\eta)]_{\xi,\eta\in\mathcal{A}_F^0}$. By Lemma 4.2 below, M_3 is nonsingular and does not depend on the size or shape of F. We have now uniquely determined all coefficients corresponding to domain points on $R_{13}(v_T)$.

We now examine coefficients corresponding to domain points on the shell $R_{12}(v_T)$. Let $F := \langle v_1, v_2, v_3\rangle$ be a face of this shell as shown in Fig. 1 (mid). We can consider the coefficients corresponding to domain points on F to be the coefficients $c_\xi^{F,12}$ of a bivariate polynomial of degree 12. The coefficients corresponding to the black dots and to the triangles are already uniquely determined as they lie either in the 5-disks around the vertices of F or the 2-tubes around its edges. We are left with 10 coefficients corresponding to the domain points $\xi\in\mathcal{A}_F^1$ marked with $\oplus$ in Fig. 1 (mid). Now if $(\alpha_1,\alpha_2,\alpha_3,\alpha_4)$ with $\alpha_1+\alpha_2+\alpha_3+\alpha_4=0$ are the direction coordinates relative to the tetrahedron $\langle v_T, v_1, v_2, v_3\rangle$ describing the unit vector perpendicular to F and pointing into T, then

$$D_F s = 13 \sum_{i+j+k=12} (\alpha_1 c_{ijk}^{F,12} + \alpha_2 c_{i+1,j,k}^{F,13} + \alpha_3 c_{i,j+1,k}^{F,13} + \alpha_4 c_{i,j,k+1}^{F,13}) B_{ijk}^{F,12},$$

Setting $\{\lambda s\}_{\lambda\in\mathcal{N}_F^1}$ leads to a linear system of 10 equations for the $\{c_\xi^{F,12}\}_{\xi\in\mathcal{A}_F^1}$ with matrix $M_{10} := [B_\xi^{F,12}(\eta)]_{\xi,\eta\in\mathcal{A}_F^1}$. By Lemma 4.2, M_{10} is nonsingular and is independent of the size and shape of F. We have now shown that all coefficients corresponding to domain points on the shell $R_{12}(v_T)$ are uniquely determined.

We next examine coefficients corresponding to domain points on the shell $R_{11}(v_T)$. Let $F := \langle v_1, v_2, v_3\rangle$ be a face of this shell as shown in Fig. 1 (right). We can consider the coefficients corresponding to domain points on F to be the coefficients $c_\xi^{F,11}$ of a bivariate polynomial of degree 11. The coefficients corresponding to the black dots and to the triangles are already uniquely determined as they lie either in the 4-disks around the vertices of F or the 1-tubes around its edges. We are left with 18 coefficients corresponding to the domain points $\xi\in\mathcal{A}_F^2$ marked with $\oplus$ in Fig. 1 (right). Examining the formula for $D_F^2 s$, it is easy to see that setting $\{\lambda s\}_{\lambda\in\mathcal{N}_F^2}$ leads to an 18×18 system of equations for these coefficients with matrix $M_{18} := [B_\xi^{F,11}(\eta)]_{\xi,\eta\in\mathcal{A}_F^2}$. By Lemma 4.2, M_{18} is nonsingular and is independent of the size and shape of F. We have now shown that all coefficients corresponding to domain points on the shell $R_{11}(v_T)$ are uniquely determined.

To show that the coefficients of s corresponding to the remaining domain points in T_{CT} are uniquely determined, we note that by the C^{12} smoothness at v_T, we may consider the B-coefficients of s corresponding to domain points in the ball $D_{12}(v_T)$ as those of a polynomial g of degree 12 which has been subdivided with split point v_T. The space $\mathcal{P}_{12}^3$ has dimension 455. Let c_{ijkl}^T be the B-coefficients of g corresponding to the domain points in $\mathcal{D}_{T,12}$. Note that $\mathcal{D}_{T,12}$ is not the same as $\mathcal{D}_{T_{CT},12}$. By the above, we have already uniquely determined the coefficients of g corresponding to domain points in $\mathcal{D}_{T,12}$ in balls of radius 5 around each vertex of T, in tubes of radius 2 around each edge, and on the faces of the shells $R_{12}(v_T)$ and $R_{11}(v_T)$. Thus, a total of $4\times 56+6\times 14+4\times 10+4\times 18 = 420$ coefficients are already determined. Since the space $\mathcal{P}_{12}^3$ has dimension 455, this leaves 35 undetermined coefficients. These coefficients do not enter into the computation of any of the values λs for $\lambda \in \mathcal{N} \setminus \mathcal{N}_{v_T}$. By Lemma 4.3, they are uniquely determined by $\{\lambda s\}_{\lambda\in\mathcal{N}_{v_T}}$, and can be computed from a nonsingular system of 35 linear equations whose matrix M_{35} is independent of the size and shape of T.

Now that we know that $\mathcal{N}$ is a nodal minimal determining set for $\mathcal{S}_2(T_{CT})$, to compute the dimension of $\mathcal{S}_2(T_{CT})$ we need only compute the cardinality of $\mathcal{N}$. It is easy to see that the cardinalities of the sets $\mathcal{N}_v$, $\mathcal{N}_e$, $\mathcal{N}_F^0$, $\mathcal{N}_F^1$, $\mathcal{N}_F^2$, $\mathcal{N}_{v_T}$ are 84, 20, 3, 10, 18, and 35, respectively. Since T has four vertices, six edges, and four faces, it follows that $\#\mathcal{N} = 4 \times 84 + 6 \times 20 + 4 \times 31 + 35 = 615$. □

We now establish that our construction provides a C^2 macro element. Let $\triangle$ be an arbitrary tetrahedral partition of a polyhedral domain Ω, and let $\mathcal{V}$, $\mathcal{E}$, and $\mathcal{F}$ be its sets of vertices, edges, and faces, respectively. We assume each face F has been assigned an orientation so that the corresponding normal derivative D_F is well-defined. Let $\triangle_{CT}$ be the refined partition obtained by applying the Clough-Tocher split to each tetrahedron in $\triangle$. Let

$$\begin{aligned}\mathcal{S}_2(\triangle_{CT}) := \{s \in C^2(\Omega) : s|_{\widetilde{T}} \in \mathcal{P}_{13}^3 \text{ all } \widetilde{T} \in \triangle_{CT},\\ s \in C^3(e), \text{ for all } e \in \mathcal{E},\\ s \in C^6(v), \text{ for } v \in \mathcal{V},\\ s \in C^{12}(v_T), \text{ for all } T \in \triangle\},\end{aligned} \tag{3.5}$$

where for each $T \in \triangle$, v_T is the split point in T. Finally, let V, E, F be the cardinalities of the sets $\mathcal{V}$, $\mathcal{E}$, and $\mathcal{F}$, respectively, and let N_T be the number of tetrahedra in $\triangle$.

Theorem 3.2. *The space $\mathcal{S}_2(\triangle_{CT})$ has dimension*

$$n := 84V + 20E + 31F + 35N_T.$$

Moreover, the set

$$\mathcal{N} := \bigcup_{v\in\mathcal{V}} \mathcal{N}_v \cup \bigcup_{e\in\mathcal{E}} \mathcal{N}_e \cup \bigcup_{F\in\mathcal{F}} (\mathcal{N}_F^0 \cup \mathcal{N}_F^1 \cup \mathcal{N}_F^2) \cup \bigcup_{T\in\mathcal{T}} \mathcal{N}_{v_T} \tag{3.6}$$

is a nodal minimal determining set for $\mathcal{S}_2(\triangle_{CT})$*, where* $\mathcal{N}_v$, $\mathcal{N}_e$, $\mathcal{N}_F^0$, $\mathcal{N}_F^1$, $\mathcal{N}_F^2$, *and* $\mathcal{N}_{v_T}$ *are as in Theorem 3.1.*

Proof: It follows from Theorem 3.1 that for each tetrahedron $T \in \triangle$, the nodal data uniquely determines a spline $s_T \in \mathcal{S}_2(T_{CT})$. We now show that the s_T join together smoothly to form a spline $s \in \mathcal{S}_2(\triangle_{CT})$. Suppose that T and $\widetilde{T}$ are two tetrahedra in $\triangle_{CT}$ which share an edge $e := \langle u, v\rangle$ of $\triangle$. Let $p := s_T|_e$ and $\tilde{p} := s_{\widetilde{T}}|_e$. These are both univariate polynomials of degree 13 on e. Since the coefficients of both are computed from common nodal data at points on e, it follows that $p \equiv \tilde{p}$, and we conclude that s and $\tilde{s}$ join with C^0 continuity along the edge e. A similar argument shows that for all α with $|\alpha| \le 3$, the univariate polynomials $D^{\alpha}_{e,1} s_T|_e$ and $D^{\alpha}_{e,1} s_{\widetilde{T}}|_e$ also agree on e since they are constructed from common nodal data at points along e.

Now suppose T and $\widetilde{T}$ share a common face F. Then by construction, all B-coefficients of the bivariate polynomials $g := s_T|_F$ and $\tilde{g} := s_{\widetilde{T}}|_F$ agree, and we conclude that g and $\tilde{g}$ join continuously across the face F. A similar argument shows that the bivariate polynomials $D_F s_T|_F$ and $D_F s_{\widetilde{T}}|_F$ also agree on F due to the fact that both polynomials are computed from common nodal data at points on F. The same holds for the derivatives $D_F^2 s_T|_F$ and $D_F^2 s_{\widetilde{T}}|_F$.

We have now shown that the nodal data $\mathcal{N}$ uniquely determines a spline $s \in \mathcal{S}_2(\triangle_{CT})$, and thus is a nodal minimal determining set for $\mathcal{S}_2(\triangle_{CT})$. $\square$

Theorem 3.2 shows that for any function $f \in C^6(\Omega)$, there is a unique spline $s \in \mathcal{S}_2(\triangle_{CT})$ solving the Hermite interpolation problem

$$\lambda s = \lambda f, \qquad \text{for all } \lambda \in \mathcal{N},$$

or equivalently,

1) $D^{\alpha} s(v) = D^{\alpha} f(v)$, for all $|\alpha| \le 6$ and all $v \in \mathcal{V}$,
2) $D_e^{\beta} s(\eta^i_{e,j}) = D_e^{\beta} f(\eta^i_{e,j})$, for all $|\beta| = i$ with $1 \le j \le i$ and $1 \le i \le 3$, and for all edges e of $\triangle$,
3) $s(\xi) = f(\xi)$ for all $\xi \in A_F^0$ and all faces F of $\triangle$,
4) $D_F s(\xi) = D_F f(\xi)$ for all $\xi \in A_F^1$ and all faces F of $\triangle$,
5) $D_F^2 s(\xi) = D_F^2 f(\xi)$ for all $\xi \in A_F^2$ and all faces F of $\triangle$,
6) $s(\xi) = f(\xi)$ for all $\xi \in \mathcal{A}_T$ and all $T \in \triangle$.

The mapping which takes functions $f \in C^6(\Omega)$ to this Hermite interpolating spline defines a linear operator $\mathcal{I}_{CT} : C^6(\Omega) \to \mathcal{S}_2(\triangle_{CT})$. The construction guarantees that $\mathcal{I}_{CT} s = s$ for all $s \in \mathcal{S}_2(\triangle_{CT})$, and in particular for all $p \in \mathcal{P}^3_{13}$. It is clear from the construction that the computation of the B-coefficients of the interpolating spline s is local. More precisely, for every domain point ξ, the corresponding coefficient c_ξ of s depends only on values of f and its derivatives at points Γ_ξ in star(T), where $T \in \triangle$ is a tetrahedron containing ξ.

For the remainder of this section we assume that for each tetrahedron $T := \langle v_1, v_2, v_3, v_4 \rangle \in \triangle$, the split point is taken to be $v_T = (v_1+v_2+v_3+v_4)/4$, i.e., the centroid or barycenter of T. Let $\kappa := \max_{T\in\triangle} R_T/r_T$, where r_T and R_T are the radii of the inscribed and circumscribed spheres associated with T, respectively. We now show that the computation of the B-coefficients of $s := \mathcal{I}_{CT} f$ is stable in the sense that there exists a constant C depending only on κ such that if $\xi \in \mathcal{D}_{\triangle_{CT},d} \cap T$, then

$$|c_\xi| \le C \sum_{i=1}^{6} |\Omega_T|^i |f|_{i,\text{star}(T)}, \tag{3.7}$$

where Ω_T is the union of the tetrahedra in star(T). Here

$$|f|_{i,B} := \sum_{|\alpha|=i} \|D^\alpha f\|_B, \tag{3.8}$$

for any compact subset B of Ω, where we write $\|\cdot\|_B$ for the infinity norm. Indeed, the bound (3.7) is clear for all domain points in balls of the form $D_6(v)$ around vertices of $\triangle$ by the well-known connection between B-coefficients in such a ball and derivatives at v. A similar argument applies to all domain points in tubes of radius 3 around edges. As shown in the proof of Theorem 3.1, the coefficients of s which are determined from the functionals in the sets $\mathcal{N}_f^0$, $\mathcal{N}_F^1$, and $\mathcal{N}_F^2$ are obtained by solving linear systems of equations associated with fixed matrices M_3, M_{10}, and M_{18}. The coefficients which are determined from the functionals in the sets $\mathcal{N}_{v_T}$ are obtained by solving linear systems of equations with the matrix M_{35}, followed by subdivision about the split point v_T, which is also a stable process. It follows that (3.7) holds for all coefficients of s.

Using standard arguments (cf. [15]) we can now establish an optimal order error bound for functions in the classical Sobolev spaces $W_\infty^m(\Omega)$. Let $|\triangle|$ be the mesh size of $\triangle$, i.e., the maximum diameter of the tetrahedra in $\triangle$.

Theorem 3.3. *There exists a constant K depending only κ such that for every $f \in C^m(\Omega)$ with $6 \le m \le 13$,*

$$\|D^\alpha(f - \mathcal{I}_{CT} f)\|_\Omega \le K|\triangle|^{m+1-|\alpha|}|f|_{m+1,\Omega}, \tag{3.9}$$

for all $|\alpha| \le m$.

Proof: Since the proof is similar to the proof of Theorem 6.2 in [15] (see also [12,13] for similar arguments in the bivariate case), we can be brief. Fix $T \in \triangle$, and let $f \in W_\infty^{m+1}(\Omega)$. Fix α with $|\alpha| \le m$. By Lemma 4.3.8 of [5], there exists a polynomial $q := q_{f,T} \in \mathcal{P}_{13}^3$ such that

$$\|D^\alpha(f-q)\|_{\Omega_T} \le |(f-q)|_{|\alpha|,\Omega_T} \le K_1|\Omega_T|^{m+1-|\alpha|}|f|_{m+1,\Omega_T}, \tag{3.10}$$

where Ω_T is the union of the tetrahedra in star(T). Since $\mathcal{I}_{CT} p = p$ for all $p \in \mathcal{P}_{13}^3$,

$$\|D^\alpha(f - \mathcal{I}_{CT} f)\|_T \le \|D^\alpha(f-q)\|_T + \|D^\alpha \mathcal{I}_{CT}(f-q)\|_T.$$

It suffices to estimate the second quantity. Applying the Markov inequality [18] to each of the polynomials $\mathcal{I}_{CT}(f-q)|_{T_j}$, where $T_1, \ldots, T_4$ are the tetrahedra in the CT-split of T, we have

$$\|D^\alpha \mathcal{I}_{CT}(f-q)\|_{T_j} \le K_2 |\triangle|^{-|\alpha|} \|\mathcal{I}_{CT}(f-q)\|_{T_j},$$

where K_2 is a constant depending only on κ. Let c_ξ be the B-coefficients of the polynomial $\mathcal{I}_{CT}(f-q)|_{T_j}$ relative to the tetrahedron T_j. Then combining (3.7) with the fact that the Bernstein basis polynomials form a partition of unity, it is easy to see that

$$\|\mathcal{I}_{CT}(f-q)\|_{T_j} \le K_3 \max_{\xi \in \mathcal{D}_{T_j,d}} |c_\xi| \le K_4 \sum_{i=0}^{6} |\Omega_T|^i |f-q|_{i,\Omega_T}.$$

Taking the maximum over j and combining this with (3.10) gives

$$\|\mathcal{I}_{CT}(f-q)\|_T \le K_5 |\triangle|^{m+1} |f|_{m+1,\Omega_T},$$

which gives

$$\|D^\alpha(f - \mathcal{I}_{CT} f)\|_T \le K_6 |\triangle|^{m+1-|\alpha|} |f|_{m+1,\Omega_T}.$$

Finally, we take the maximum over all tetrahedra T in $\triangle$ to get (3.9). □

§4. Polynomial Interpolation in Bernstein–Bézier Form

In this section we present two lemmas on interpolation by polynomials which were needed above. We first recall a conjecture of the second author concerning interpolation with bivariate Bernstein basis polynomials.

Conjecture 4.1. [14] *Given d and a triangle $F := \langle v_1, v_2, v_3 \rangle$, let Γ be an arbitrary subset of $\mathcal{D}_{F,d}$. Then the matrix*

$$M := [B_\xi^{F,d}(\eta)]_{\xi,\eta \in \Gamma} \tag{4.1}$$

is nonsingular, and in fact has a positive determinant. Thus, for any real numbers $\{z_\eta\}_{\eta\in\Gamma}$, there is a unique $p := \sum_{\xi\in\Gamma} c_\xi B_\xi^{F,d}$ such that $p(\eta) = z_\eta$ for all $\eta \in \Gamma$.

Discussion: Since the entries of M depend only on barycentric coordinates, it follows that M does not depend on the size or shape of F. It is easy to give a direct proof for $d \le 3$. The conjecture has also been verified for $d \le 7$ numerically, see [13,12]. It has also been proved for various special configurations of Γ, see [11]. □

Here we need the following special case of this conjecture.

Lemma 4.2. *The above conjecture holds for the sets*

1) $\Gamma := \mathcal{A}_F^0 \subset \mathcal{D}_{F,13}$,
2) $\Gamma := \mathcal{A}_F^1 \subset \mathcal{D}_{F,12}$,
3) $\Gamma := \mathcal{A}_F^2 \subset \mathcal{D}_{F,11}$.

Proof: The claim can be easily checked numerically. Alternatively, we can establish it directly in each case by removing common factors from the rows and columns of M to reduce it to a matrix which can easily be seen to have a positive determinant. □

We also need the following result on interpolation using linear combinations of trivariate Bernstein basis polynomials.

Lemma 4.3. *Given* $T := \langle v_1, v_2, v_3, v_4 \rangle$, *let* $\Gamma := \{\xi_{ijkl}^{T,12} : i,j,k,l \geq 2\}$. *Then the matrix*

$$M := [B_\xi^{T,12}(\eta)]_{\xi,\eta\in\Gamma} \tag{4.2}$$

is nonsingular, and for any $\{z_\eta\}_{\eta\in\Gamma}$, *there is a unique* $p := \sum_{\xi\in\Gamma} c_\xi B_\xi^{T,12}$ *such that* $p(\eta) = z_\eta$ *for all* $\eta \in \Gamma$.

Proof: The interpolation conditions lead to a 35×35 matrix M_{35} whose entries are independent of the size or shape of T. Thus, the fact that M_{35} is nonsingular could be verified numerically, but instead we give the following direct proof. Suppose that $p(\eta) := \sum_{\xi\in\Gamma} c_\xi B_\xi^{T,12}(\eta) = 0$ for $\eta \in \Gamma$. To complete the proof it suffices to show that $p \equiv 0$. By properties of the $B_{ijkl}^{T,12}$, it is clear that p must vanish on the faces of T, and thus there exists a polynomial $p_8 \in \mathcal{P}_8^3$ such that $p = \ell_1\ell_2\ell_3\ell_4 p_8$, where for each i, ℓ_i is the linear polynomial which vanishes on the i-th face of T. A further examination of the properties of the $B_{ijkl}^{T,12}$ shows that p_8 must also vanish on the outer faces of T, and we have $p_8 = \ell_1\ell_2\ell_3\ell_4 p_4$, where $p_4 \in \mathcal{P}_4^3$. But now the condition $p(\eta) = 0$ for $\eta \in \Gamma$ implies $p_4(\eta) = 0$ for $\eta \in \Gamma$, and it follows that $p_4 \equiv 0$ which in turn implies that $p \equiv 0$. □

§5. Remarks

Remark 1. In the bivariate setting, there has been a lot of work on C^r macro-elements on various splits, see e.g. [4,3,9,10], and references therein.

Remark 2. C^r trivariate polynomial macro-elements defined on nonsplit tetrahedra were constructed in [21] using polynomials of degree $8r+1$. If used to construct a Hermite interpolant associated with a general tetrahedral partition, they produce a superspline with C^{2r} supersmoothness around edges, and C^{4r} supersmoothness at vertices.

Remark 3. C^1 trivariate macro-elements were constructed on the CT-split using splines of degree 5 in [1], and on the WF-split using splines of degree 3 in [19]. C^1 macro-elements were also constructed on a split involving 24 tetrahedra using splines of degree 2 in [20], although their use in practice for partitions $\triangle$ involving more than one tetrahedron requires some rather severe geometric constraints. Recently, C^1 macro-elements were developed for a split of a rectangular box into 24 tetrahedra, using splines of degree 5, see [15]. C^1 macro-elements based on octahedral partitions were developed in [7].

Remark 4. By examining slices through T_{CT}, it can be shown that it is not possible to construct C^2 macro-elements on the CT-split using splines with smoothness less than 3 around the edges or smoothness 4 at the vertices. This in turn implies that 13 is the minimal degree possible.

Remark 5. The java code of the first author for examining determining sets for piecewise polynomial functions on tetrahedral partitions was a key tool in developing the macro-elements described in this paper. The code can compute the dimension of trivariate spline spaces, find minimal determining sets, and solve the smoothness equations in exact arithmetic. It can be used or downloaded from `http://www.math.utah.edu/~pa/3DMDS`, along with associated documentation.

Remark 6. We have used the java code to explore the possibility of imposing additional smoothness conditions on our superspline space $\mathcal{S}_2(T_{CT})$ to get a space of dimension 580 which is uniquely determined by the nodal functionals of Theorem 3.1, minus the set $\mathcal{N}_{v_T}$. This would give us a C^2 macro-element which is defined by natural degrees of freedom only, i.e., information on the boundary of the tetrahedron T. However, we have not been able to find a symmetric way to do this, and expect that if it can be done at all, it would require imposing various individual smoothness conditions, as was done in the bivariate case, cf. [4,3] to get natural degrees of freedom for bivariate macro-element spaces.

Remark 7. It is possible to create macro-elements with fewer degrees of freedom by the process of condensation. This amounts to further restricting the spline space by forcing cross-derivatives along edges or through faces of the tetrahedron T to be of reduced degree. The main problem with this strategy is that it produces elements which no longer have the capability of reproducing the full polynomial space, and thus have reduced approximation power.

Remark 8. In this paper we have given error bounds for Hermite interpolation with our macro element in the uniform norm. Analogous results hold for the p-norms, and can be proved using appropriate quasi-interpolation operators, cf. Sect. 10 of [8] for the bivariate case.

Remark 9. It is relatively straightforward to check that there is a similar C^3 macro element on the CT-split of a tetrahedron which uses splines of degree 17 which are C^8 around the vertices, C^4 around the edges, and C^{15} at the centroid v_T. This space has dimension 1344, with 1228 natural degrees of freedom (nodal data at points on the face of T).

Remark 10. We have recently learned [6] that Ming-Jun Lai and Alain Le Méhauté have independently studied C^r macro-elements based on the CT split.

Remark 11. Using the java software, we have also designed C^2 macro-elements based on a trivariate analog of the Worsey-Farin split described in [19] as well as the double Clough-Tocher split of a tetrahedron which is obtained by first applying the CT-split, and then applying it again to each of the resulting four subtetrahedra. We are also working on elements based on an analog of the bivariate split described in [17]. We will report on these results elsewhere.

Remark 12. It is believed [14] that the analog of Conjecture 4.1 also holds for Bernstein basis polynomials on simplices in any number of variables. In the one-variable case, this follows immediately from the fact that the univariate Bernstein basis polynomials form a complete Tchebycheff system. For tetrahedra, the conjecture asserts that the matrices $M := [B_\xi^{T,d}(\eta)]_{\xi,\eta\in\Gamma}$ are nonsingular for all choices of $\Gamma \in \mathcal{D}_{T,d}$, and Lemma 4.3 is just a special case.

Remark 13. It is possible to replace the set of functionals $\mathcal{N}_{v_T}$ in Theorem 3.1 by the set $\{\varepsilon_{v_T} D^\alpha\}_{|\alpha|\le 4}$, which corresponds to Hermite interpolation at the point v_T.

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