A C^2 Trivariate Double-Clough-Tocher Macro-Element

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

§1. Introduction

This paper is a companion to our recent papers [6,7] in which we constructed C^2 trivariate macro-elements based on the Clough-Tocher and Worsey-Farin splits of a tetrahedron. The Clough-Tocher split involves four subtetrahedra, and the corresponding element makes use of supersplines of degree 13. The Worsey-Farin split involves twelve subtetrahedra, but admits the construction of a macro-element using supersplines of degree 9. The purpose of this paper is to describe another C^2 macro-element which works with polynomials of degree 9, but which is based on the double-Clough-Tocher split (see Sect. 3 below) which involves sixteen tetrahedra. While our construction here involves more subtetrahedra than the Worsey-Farin split, out new element has fewer degrees of freedom and does not require splitting faces of tetrahedra, thereby avoiding potential problems with stability.

We recall [6,7] that a trivariate macro-element defined on a tetrahedron T consists 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 $i = 1, \ldots, n$.

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These functionals are called the nodal degrees of freedom of the element. 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 a tetrahedral partition $\triangle$, then the resulting piecewise function is C^r continuous globally. Our aim here is to construct a C^2 macro-element.

The paper is organized as follows. In Sect. 2 we present some background material and notation. The construction of our macro-element for a single tetrahedron is presented in Sect. 3, where we identify the dimension of the resulting macro-element space and give a minimal determining set for it. The macro-element space for a double-Clough-Tocher refinement of an arbitrary tetrahedral partition is discussed in Sect. 4, where we give a dimension statement and an explicit minimal determining set. Sect. 5 is devoted to the construction of a nodal determining set for our macro-element space, and the study of an associated Hermite interpolation operator, including an error bound. We conclude the paper with a number of remarks.

§2. Preliminaries

Throughout the paper, we follow the notation of our earlier papers [6,7], but for completeness repeat some of the key ideas. We write $\mathcal{P}_d^j$ for the $\binom{d+j}{j}$ dimensional linear space of polynomials of degree d in j variables. In dealing with polynomials and splines, we will make use of well-known Bernstein–Bézier methods as described for example in [1–7,9–13,15,16]. 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 $\xi_{ijkl}^{T,d} := \frac{(iv_1+jv_2+kv_3+lv_4)}{d}$, 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 common points in neighboring tetrahedra are not repeated.

Given $\rho > 0$, we refer to the set $D_\rho(v)$ 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 set $R_\rho(v)$ of all domain points which are at a distance ρ from v as the shell of radius ρ around v. 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.

Suppose $\mathcal{S}$ is a linear subspace of $\mathcal{S}_d^0(\triangle)$, and suppose $\mathcal{M}$ is a subset of $\mathcal{D}_{\triangle,d}$. Then $\mathcal{M}$ is said to be a determining set for $\mathcal{S}$ provided that if $s \in \mathcal{S}$ and its B-coefficients satisfy $c_\xi = 0$ for all $\xi \in \mathcal{M}$, then $s \equiv 0$. It is called a minimal determining set (MDS) for $\mathcal{S}$ provided there is no smaller determining set. It is well known that $\mathcal{M}$ is a MDS for $\mathcal{S}$ if and only if setting the coefficients $\{c_\xi\}_{\xi\in\mathcal{M}}$ of a spline in $\mathcal{S}$ uniquely determines all coefficients of s. Now 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 $\mathcal{N}$ is said to be 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 there is no smaller NDS, or equivalently, 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. The Basic Macro-element on one Tetrahedron

Given a tetrahedron $T := \langle v_1, v_2, v_3, v_4\rangle$, let $v_T := (v_1+v_2+v_3+v_4)/4$ be the barycenter of T. Then connecting v_T to the vertices v_i of T results in a partition of T into four subtetrahedra $T_1,\ldots,T_4$. This gives the classical Clough-Tocher split of T used in [2,6]. Now for each $i=1,\ldots,4$, let v_T^i be the barycenter of T_i. For each $i=1,\ldots,4$, we now connect v_T^i to the vertices of T_i to split T_i into four smaller tetrahedra. This results in a partition of T into 16 subtetrahedra. In analogy to a similar partition of triangles used in [1], we call this partition the double-Clough-Tocher split of T and denote it by T_{DCT}.

We write $\mathcal{V}_T$, $\mathcal{E}_T$, and $\mathcal{F}_T$ for the sets of vertices, edges, and faces of T. Let $\mathcal{V}_T^c$ be the set of four subcenters v_T^i of the DCT-split of T. Let $\mathcal{F}_T^1$ be the set of 6 faces of T_{DCT} of the form $\langle v_T, v_i, v_j\rangle$, i.e., whose vertices include v_T and two of the vertices of T.

We now introduce our basic macro-element space as a space of super-splines defined on T_{DCT}:

$$\begin{aligned}\mathcal{S}_2(T_{DCT}) := \{s\in C^2(T):\ & s|_t\in\mathcal{P}_9^3 \text{ all } t\in T_{DCT},\\ & s\in C^4(v),\ \text{for all } v\in\mathcal{V}_T,\\ & s\in C^7(v_T),\\ & s\in C^8(v),\ \text{for all } v\in\mathcal{V}_T^c,\\ & s\in C^3(F),\ \text{for all } F\in\mathcal{F}_T^1\}.\end{aligned}\tag{1}$$

As usual, if v is a vertex of T_{DCT}, 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_{DCT}, then $s\in C^\mu(e)$ means that all polynomial pieces of s defined on tetrahedra sharing the edge e have common derivatives up to order μ on e. Similarly, if F is a face of T_{DCT}, then $s\in C^\mu(F)$ means that all polynomial pieces of s defined on tetrahedra sharing the face F have common derivatives up to order μ on F.

Before proceeding, we first make some remarks about our fairly complicated definition of $\mathcal{S}_2(T_{DCT})$. The construction is the result of a considerable amount of experimentation with the first author's java code for working with trivariate splines, see Remark 7. In creating $\mathcal{S}_2(T_{DCT})$, we had two aims in mind: to create a macro-element which will be globally C^2 smooth, and to minimize the complexity and number of degrees of freedom. First, we observe that we are forced to impose the C^4 supersmoothness at the vertices of T since otherwise we could not make macro-elements on adjoining tetrahedra join with C^2 smoothness, see Remark 6. Since derivatives up to order 4 at the vertices are not allowed to interfere (or equivalently, balls of radius 4 around the vertices are not allowed to overlap), this forces us to use polynomials of degree (at least) nine. The additional supersmoothness in the definition of $\mathcal{S}_2(T_{DCT})$ has been imposed in order to remove unnecessary degrees of freedom from our macro-element. After checking all possible variations of supersmoothness at vertices, around edges, and across faces, we found that the present space has the minimal number of degrees of freedom achievable without resorting to imposing individual special smoothness conditions.

For each vertex v of T_{DCT}, let T_v be one of the tetrahedra in T_{DCT} attached to v. For each edge $e := \langle u, v \rangle$ of T, let T_e be one of the four tetrahedra containing e, and let $E_2(e)$ denote the set of domain points in the tube of radius 2 around e which do not lie in the disks $D_4(u)$ or $D_4(v)$. Finally, for each face $F := \langle v_1, v_2, v_3 \rangle$ of T, let $T_F := \langle w, v_1, v_2, v_3 \rangle$ with $w \in \mathcal{V}_T^c$ be the tetrahedron in T_{DCT} containing F.

The results of this paper are based on the following

Theorem 1. *The space $\mathcal{S}_2(T_{DCT})$ has dimension 280. Moreover,*

$$\mathcal{M} := \bigcup_{v \in \mathcal{V}_T} \mathcal{M}_v \cup \bigcup_{e \in \mathcal{E}_T} \mathcal{M}_e \cup \bigcup_{F \in \mathcal{F}_T} \left[\mathcal{M}_F^0 \cup \mathcal{M}_F^1 \cup \mathcal{M}_F^2\right] \cup \mathcal{M}_T \tag{2}$$

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

1) $\mathcal{M}_v := D_4(v) \cap T_v$,

2) $\mathcal{M}_e := E_2(e) \cap T_e$,

3) $\mathcal{M}_F^0 := \{\xi_{0333}^{T_F,9}\}$,

4) $\mathcal{M}_F^1 := \{\xi_{1ijk}^{T_F,9} : i, j, k \geq 2, \}$

5) $\mathcal{M}_F^2 := \{\xi_{2ijk}^{T_F,9} : i, j, k \geq 1\} \setminus \{\xi_{2115}^{T_F,9}, \xi_{2151}^{T_F,9}, \xi_{2511}^{T_F,9}\}$,

6) $\mathcal{M}_T := \bigcup_{i=1}^4 \left[D_1(v_T^i) \cap T_{v_T^i}\right]$.

Proof: We have verified that $\dim \mathcal{S}_2(T_{DCT}) = 280$ and that $\mathcal{M}$ is a MDS using the java program described in Remark 7, working in exact arithmetic. As a check on the MDS computation, we can compute the cardinality of $\mathcal{M}$. The cardinalities of the sets $\mathcal{M}_v$, $\mathcal{M}_e$, $\mathcal{M}_F^0$, $\mathcal{M}_F^1$, $\mathcal{M}_F^2$, and $\mathcal{M}_T$ are 35, 8, 1, 6, 12, and 16, respectively. Since T has 4 vertices, 6 edges, and 4 faces, we find that $\#\mathcal{M} = 4\times 35+6\times 8+4\times(1+6+12)+16 = 280$. □

§4. The Macro-element Space $\mathcal{S}_2(\triangle_{DCT})$

We now show that the construction of the previous section can be used to define a C^2 macro-element space starting with an arbitrary tetrahedral partition $\triangle$ of a polyhedral domain Ω. Let $\triangle_{DCT}$ be the refined partition obtained by applying the double-Clough-Tocher split to each tetrahedron in $\triangle$. Let $\mathcal{V}$, $\mathcal{E}$, and $\mathcal{F}$ be the sets of vertices, edges, and faces of $\triangle$, respectively. We write n_V, n_E, n_F for the cardinalities of these sets. We denote the number of tetrahedra in $\triangle$ by n_T. Let

$$\mathcal{F}^1 := \bigcup_{T\in\triangle} \mathcal{F}_T^1, \qquad \mathcal{V}^c := \bigcup_{T\in\triangle} \mathcal{V}_T^c,$$

where $\mathcal{F}_T^1$ and $\mathcal{V}_T^c$ are as in Sect. 3. We are now ready to define a DCT-macro-element space defined on $\triangle_{DCT}$:

$$\begin{aligned} \mathcal{S}_2(\triangle_{DCT}) := \{s \in C^2(\Omega):\ & s|_t \in \mathcal{P}_9^3 \text{ all } t \in \triangle_{DCT}, \\ & s \in C^4(v), \text{ for all } v \in \mathcal{V}, \\ & s \in C^7(v_T), \text{ for all } T \in \triangle, \\ & s \in C^8(v), \text{ for all } v \in \mathcal{V}^c, \\ & s \in C^3(F), \text{ for all } F \in \mathcal{F}^1\}. \end{aligned} \tag{3}$$

To define a MDS for $\mathcal{S}_2(\triangle_{DCT})$ we need some more notation. For each vertex v of $\triangle_{DCT}$, let T_v be one of the tetrahedra in $\triangle_{DCT}$ attached to v. For each edge $e := \langle u, v\rangle$ of $\triangle$, let T_e be one of the tetrahedra in $\triangle_{DCT}$ containing e, and let $E_2(e)$ denote the set of domain points in the tube of radius 2 around e which do not lie in the balls $D_4(u)$ or $D_4(v)$. Finally, for each face F of T, let $T_F := \langle w, v_1, v_2, v_3\rangle$ be a tetrahedron in $\triangle_{DCT}$ containing F.

Theorem 2. *The space $\mathcal{S}_2(\triangle_{DCT})$ has dimension $35n_V + 8n_E + 19n_F + 16n_T$, and the set*

$$\mathcal{M} := \bigcup_{v\in\mathcal{V}} \mathcal{M}_v \cup \bigcup_{e\in\mathcal{E}} \mathcal{M}_e \cup \bigcup_{F\in\mathcal{F}} [\mathcal{M}_F^0 \cup \mathcal{M}_F^1 \cup \mathcal{M}_F^2] \cup \bigcup_{T\in\triangle} \mathcal{M}_T \tag{4}$$

is a minimal determining set for $\mathcal{S}_2(\triangle_{DCT})$, where

1) $\mathcal{M}_v := D_4(v) \cap T_v$,

2) $\mathcal{M}_e := E_2(e) \cap T_e$,

3) $\mathcal{M}_F^0 := \{\xi_{0333}^{T_F,9}\}$,

4) $\mathcal{M}_F^1 := \{\xi_{1ijk}^{T_F,9} : i,j,k \ge 2\}$

5) $\mathcal{M}_F^2 := \{\xi_{2ijk}^{T_F,9} : i,j,k \ge 1\} \setminus \{\xi_{2115}^{T_F,9}, \xi_{2151}^{T_F,9}, \xi_{2511}^{T_F,9}\}$,

6) $\mathcal{M}_T := \bigcup_{i=1}^4 \left[D_1(v_T^i) \cap T_{v_T^i}\right]$.

Proof: We shall show that $\mathcal{M}$ is a MDS for $\mathcal{S}_2(\triangle_{DCT})$. This implies that the dimension of $\mathcal{S}_2(\triangle_{DCT})$ is just the cardinality of $\mathcal{M}$, which is easily seen to be equal to the given formula.

To show that $\mathcal{M}$ is a minimal determining set for $\mathcal{S}_2(\triangle_{DCT})$, we need to show that if $s \in \mathcal{S}_2(\triangle_{DCT})$, then we can set the coefficients $\{c_\xi\}_{\xi\in\mathcal{M}}$ to *arbitrary* values, and all other coefficients will be *uniquely* determined. First, since the balls $D_4(v)$ do not overlap, it is clear that we can set all of the coefficients corresponding to the sets $\mathcal{M}_v$ to arbitrary values, and then by the C^4 smoothness at vertices, all other coefficients corresponding to domain points in balls $D_4(v)$ will be uniquely determined. Similarly, since the sets $E_2(e)$ do not overlap each other or any of the balls $D_4(v)$, we can set all of the coefficients corresponding to the sets $\mathcal{M}_e$ to arbitrary values, and then by the C^2 smoothness of s, all other coefficients corresponding to domain points in the sets $E_2(e)$ will be uniquely determined.

Now let F be a face of a tetrahedron $T \in \triangle$, and let $T_F \in \triangle_{DCT}$ be the tetrahedron associated with F in the definition of $\mathcal{M}_F^0$, $\mathcal{M}_F^1$, and $\mathcal{M}_F^2$. Suppose we set the coefficients of $s|_{T_F}$ corresponding to $\mathcal{M}_F^0 \cup \mathcal{M}_F^1 \cup \mathcal{M}_F^2$. Suppose now that F is an interior face of $\triangle$, and let $\widetilde{T}_F$ be the other tetrahedron in $\triangle_{DCT}$ which shares the face F. Then the coefficients of $s|_{\widetilde{T}_F}$ corresponding to domain points in $\widetilde{T}$ which lie within a distance of 2 of F are uniquely determined from the C^2 smoothness across F. In particular, this uniquely determines the coefficients of $s|_{\widetilde{T}_F}$ corresponding to domain points in the analogous set $\widetilde{\mathcal{M}}_F^0 \cup \widetilde{\mathcal{M}}_F^1 \cup \widetilde{\mathcal{M}}_F^2$ associated with $\widetilde{T}_F$.

For each tetrahedron T in $\triangle_{DCT}$, we have now uniquely determined all of the coefficients of s corresponding to domain points in the minimal determining set of Theorem 1 for $s|_T$. Thus s is uniquely determined on each T, and thus everywhere. $\square$

§5. A Nodal MDS and Hermite Interpolation

In this section we show how to construct a nodal minimal determining set for the macro-element space of the previous section, and then use it to solve a certain Hermite interpolation problem. First we need some additional notation.

Given any multi-index $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, we write D^α for the partial derivative $D_x^{\alpha_1} D_y^{\alpha_2} D_z^{\alpha_3}$. 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 represents 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 equally spaced points in the interior of e:

$$\eta_{e,j}^i := \frac{(i-j+1)u + jv}{i+1}, \qquad j = 1, \ldots, i, \tag{5}$$

for all $i > 0$. Given a point $\eta \in \mathbb{R}^3$, we write ε_η for the point-evaluation functional associated with η, so that for any trivariate function, $\varepsilon_\eta f := f(\eta)$.

For each face $F := \langle v_1, v_2, v_3 \rangle$ of $\triangle$, let D_F be the directional derivative associated with a unit normal vector to F, and let

$$\begin{aligned} A_F^1 &:= \{\xi_{ijk}^{F,8} : \ i,j,k \ge 2\}, \\ A_F^2 &:= \{\xi_{ijk}^{F,7} : \ i,j,k \ge 1\} \setminus \{\xi_{115}^{F,7}, \xi_{151}^{F,7}, \xi_{511}^{F,7}\}, \end{aligned} \tag{6}$$

where $\xi_{ijk}^{F,d} := \frac{iv_1 + jv_2 + kv_3}{d}$. We emphasize that all of these points are on the face F, and are not inside any tetrahedron. Note that there are 6 points in A_F^1 and twelve points in A_F^2.

Theorem 3. *The set*

$$\mathcal{N} := \bigcup_{v \in \mathcal{V}} \mathcal{N}_v \cup \bigcup_{e \in \mathcal{E}} \mathcal{N}_e \cup \bigcup_{F \in \mathcal{F}} [\mathcal{N}_F^0 \cup \mathcal{N}_F^1 \cup \mathcal{N}_F^2] \cup \bigcup_{T \in \triangle} \mathcal{N}_T \tag{7}$$

is a stable nodal minimal determining set for $\mathcal{S}_2(\triangle_{DCT})$, where

1) $\mathcal{N}_v := \{\varepsilon_v D^\alpha\}_{|\alpha| \le 4}$,
2) $\mathcal{N}_e := \bigcup_{i=1}^2 \bigcup_{j=1}^i \{\varepsilon_{\eta_j^i} D_e^\alpha\}_{|\alpha| = j}$,
3) $\mathcal{N}_F^0 := \{\varepsilon_{\eta_F}\}$, *where* $\eta_F = \xi_{333}^{F,9}$ *is the centroid of* F,
4) $\mathcal{N}_F^1 := \{\varepsilon_\eta D_F\}_{\eta \in A_F^1}$,
5) $\mathcal{N}_F^2 := \{\varepsilon_\eta D_F^2\}_{\eta \in A_F^2}$,
6) $\mathcal{N}_T := \bigcup_{i=1}^4 \{\varepsilon_{v_T^i} D^\alpha\}_{|\alpha| \le 1}$.

Proof: It is easy to see that the cardinality of the set $\mathcal{N}$ matches the dimension of $\mathcal{S}_2(\triangle_{DCT})$ as given in Theorem 2. We already know that the set $\mathcal{M}$ defined in that theorem is a MDS for $\mathcal{S}_2(\triangle_{DCT})$. Thus, to show that $\mathcal{N}$ is a MNDS, it suffices to show that if $s \in \mathcal{S}_2(\triangle_{DCT})$, then setting the values $\{\lambda s\}_{\lambda\in\mathcal{N}}$ determines all coefficients of s. For each $v \in \mathcal{V}$, by the C^4 smoothness at v, we can directly compute the B-coefficients corresponding to domain points in $\mathcal{M}_v := D_4(v)$ directly from the values $\{D^\alpha s(v)\}_{|\alpha|\le 4}$.

Now let $F := \langle v_1, v_2, v_3\rangle$ be a face of $\triangle$. Then for each edge $e := \langle v_i, v_{i+1}\rangle$ of F, we can use the values $\{\lambda s\}_{\lambda\in\mathcal{N}_e}$ to compute the derivatives $D_e s(\eta_1^1)$, $D_e^2 s(\eta_1^2)$, and $D_e^2 s(\eta_2^2)$, where D_e is the directional derivative corresponding to a unit vector lying in F and perpendicular to e. Now it is a standard computation to compute the B-coefficients of the bivariate spline $s|_F$ corresponding to domain points within a distance 2 of e. At this point all of the coefficients of $s|_F$ have been determined except for the coefficient corresponding to $\xi \in \mathcal{M}_F^0$. But this coefficient can now be computed directly from the value of $s(\xi_{333}^{F,9})$.

We now examine coefficients corresponding to domain points in $T_F := \langle w, v_1, v_2, v_3\rangle$, where T_F is a tetrahedron in $\triangle_{DCT}$ containing F. First we consider domain points on the shell $R_8(w)$. So far all coefficients corresponding to domain points on this shell are already known except for those corresponding to the six points in $\mathcal{M}_F^1$. These coefficients can now be computed from the values $\{D_F s(\eta)\}_{\eta\in A_F^1}$ by solving a 6×6 nonsingular linear system of equations. Next we consider the shell $R_7(w)$, where there are 12 undetermined coefficients corresponding to $\mathcal{M}_F^2$. These can be computed from the values of $\{D_F^2 s(\eta)\}_{\eta\in A_F^2}$ by solving a 12×12 nonsingular system of equations.

Now for any $v \in \mathcal{V}^c$, the coefficients of s corresponding to domain points in $D_1(v)$ can be computed directly from the values of the derivatives $\{D^\alpha s(v)\}_{|\alpha|\le 1}$. We conclude that all coefficients of s corresponding to domain points in the set $\mathcal{M}$ of Theorem 2 have been determined. The theorem then implies that all coefficients of s are determined. $\square$

Theorem 3 shows that for any function $f \in C^4(\Omega)$, there is a unique spline $s \in \mathcal{S}_2(\triangle_{DCT})$ 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 $|\alpha| \le 4$ and all $v \in \mathcal{V}$,
2) $D_e^\beta s(\eta_{e,j}^i) = D_e^\beta f(\eta_{e,j}^i)$, for all $|\beta| = i$ with $1 \le j \le i$ and $1 \le i \le 2$, and for all edges e of $\triangle$,
3) $s(\xi_{333}^{F,9}) = f(\xi_{333}^{F,9})$, for each face F of $\triangle$,
4) $D_F s(\xi) = D_F f(\xi)$ for all $\xi \in A_F^1$, for each face F of $\triangle$,

5) $D_F^2 s(\xi) = D_F^2 f(\xi)$ for all $\xi \in A_F^2$, for each face F of $\triangle$,

6) $D^\alpha s(v) = D^\alpha f(v)$, $|\alpha| \le 1$, for all $v \in \mathcal{V}^c$.

The mapping which takes functions $f \in C^4(\Omega)$ to this Hermite interpolating spline defines a linear operator $\mathcal{I}_{DCT} : C^4(\Omega) \to \mathcal{S}_2(\triangle_{DCT})$. The construction guarantees that $\mathcal{I}_{DCT} s = s$ for every spline $s \in \mathcal{S}_2(\triangle_{DCT})$, and in particular for all trivariate polynomials of degree 9. We now discuss error bounds for this interpolation process, which in turn provides an estimate for the approximation power of the space $\mathcal{S}_2(\triangle_{DCT})$. Throughout this section, we use the maximum norm. Since we want to give estimates for derivatives of splines, we will follow the usual convention in finite-element theory whereby the norm on a union of triangles Ω is taken to be the maximum of the norms over the individual triangles. We shall make use of the classical Sobolev semi-norm $|f|_{i,\Omega} = \max_{|\alpha| \le i} \|D^\alpha f\|_\Omega$.

It is well known that the key to getting error bounds for these types of spline interpolation operators is to show that the construction of the interpolating spline is both local and stable. The localness of the operator is clear from the way in which the B-coefficients of the interpolating spline s are computed. 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 in T_ξ, where $T_\xi \in \triangle$ is a tetrahedron containing ξ. Concerning stability, we have the following result.

Lemma 4. *Given a tetrahedral partition $\triangle$, let $\triangle_{DCT}$ be the corresponding double-Clough-Tocher partition, and let θ_{DCT} be the smallest angle between any two edges in $\triangle_{DCT}$ sharing a vertex. Then there exists a constant C depending only on θ_{DCT} such that for any spline $s \in \mathcal{S}_2(\triangle_{DCT})$, its coefficients satisfy*

$$|c_\xi| \le C \sum_{i=0}^{4} |T_\xi|^i |s|_{i,T_\xi}, \qquad \text{all } \xi \in \mathcal{D}_{\triangle_{DCT},9}, \tag{8}$$

where T_ξ is a tetrahedron containing ξ, and $|T_\xi|$ is its diameter.

Proof: To see that (8) holds, we review the computation of the coefficients of s as described in the proof of Theorem 3. For domain points in balls of the form $D_4(v)$ where v is a vertex of $\triangle$, (8) follows from the well-known connection between B-coefficients in such a ball and derivatives at v. In the next step we compute coefficients in the sets $\mathcal{M}_e$ from the derivatives corresponding to $\mathcal{N}_e$. For each face F, this involves converting the derivatives in $\mathcal{N}_e$ to derivatives associated with unit vectors lying in F, and then performing a standard bivariate computation. These computations are stable with a constant depending only on θ_{DCT}, and so the resulting coefficients satisfy (8).

Now for each face F of $\triangle$, we have already taken care of all coefficients corresponding to domain points lying in F, except for the one corresponding to $\xi_{333}^{F,9}$, which is determined by interpolation at this point. Since this point is the barycenter of the face, we conclude that the corresponding coefficient satisfies (8). We next examine the coefficients on $R_8(w)$ of the tetrahedron T_F in the proof of Theorem 3. These correspond to $\mathcal{M}_F^1$. To compute these coefficients, we solve a nonsingular 6×6 linear system. The matrix corresponding to this system is nonsingular and is the same for all faces. In addition, its inverse is bounded by a constant depending only on θ_{DCT}. Next we compute the 12 coefficients corresponding to $\mathcal{M}_F^2$ by solving a linear system of 12 equations whose matrix is also nonsingular and is the same for all faces. Its inverse is also bounded by a constant depending only θ_{DCT}. Since the coefficients corresponding to $\mathcal{M}_T$ are computed directly from derivatives, it follows immediately that they also satisfy (8).

At this point we have shown that (8) is satisfied for all $\xi \in \mathcal{M}$. Now all remaining coefficients are computed from smoothness conditions, and in particular, satisfy

$$|c_\xi| \le \kappa \max_{\eta \in \mathcal{M}} |c_\eta|, \qquad \text{all } \xi \in \mathcal{D}_{\triangle_{DCT},9} \setminus \mathcal{M}, \tag{9}$$

for some absolute constant κ. This follows from the fact every tetrahedron T in $\triangle$ is split in exactly the same way (using Clough-Tocher splits associated with barycenters), and all coefficients associated with domain points not in $\mathcal{M}$ are computed in the same way for each T. We conclude that (8) holds for all domain points. □

Given a tetrahedral partition $\triangle$, we write $|\triangle|$ for the diameter of the largest tetrahedron in $\triangle$.

Theorem 5. *There exists a constant K depending only on θ_{DCT} such that for every $f \in C^{m+1}(\Omega)$ with $3 \le m \le 9$,*

$$\|D^\alpha(f - \mathcal{I}_{DCT} f)\|_\Omega \le K |\triangle|^{m+1-|\alpha|} |f|_{m+1,\Omega}, \tag{10}$$

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

Proof: The proof is similar to the proofs of Theorem 3.3 in [6] and Theorem 6.3 in [7]. Fix $T \in \triangle$, and let $f \in C^{m+1}(\Omega)$. By Lemma 4.3.8 of [8], there exists a polynomial $q := q_{f,T} \in \mathcal{P}_m^3$ such that

$$\|D^\beta(f-q)\|_T \le |(f-q)|_{|\beta|,T} \le K_1 |T|^{m+1-|\beta|} |f|_{m+1,T}, \tag{11}$$

for all β with $|\beta| \le m$. Now fix α with $|\alpha| \le m$. Since $\mathcal{I}_{DCT} p = p$ for all $p \in \mathcal{P}_9^3$,

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

We can estimate the first term using (11) with $\beta = \alpha$. To estimate the second term, we now apply the Markov inequality [17] to each of the polynomials $\mathcal{I}_{DCT}(f-q)|_{T_j}$, where $T_1, \ldots, T_{16}$ are the tetrahedra in the DCT-split of T. Using the fact that $|T|/|T_j| \le 16$, we get

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

where K_2 is a constant depending only on θ_{DCT}. Let c_ξ be the B-coefficients of the polynomial $\mathcal{I}_{DCT}(f-q)|_{T_j}$ relative to the tetrahedron T_j. Then combining (8), (11), and the fact that the Bernstein basis polynomials form a partition of unity, it follows that

$$\|\mathcal{I}_{DCT}(f-q)\|_{T_j} \le \max_{\xi \in \mathcal{D}_{T_j,d}} |c_\xi| \le K_3 \sum_{i=0}^{4} |T|^i |f-q|_{i,T}.$$

Taking the maximum over j and combining this with (11) gives

$$\|\mathcal{I}_{DCT}(f-q)\|_T \le K_4 |T|^{m+1} |f|_{m+1,T},$$

which gives

$$\|D^\alpha(f - \mathcal{I}_{DCT} f)\|_T \le K_5 |T|^{m+1-|\alpha|} |f|_{m+1,T}.$$

Maximizing over all tetrahedra T in $\triangle$, we get (10). $\square$

§6. Remarks

Remark 1. In the bivariate setting, C^r macro-elements have been studied by several authors, see e.g. [1,4,5,11,12], and references therein.

Remark 2. As far as we know, double-Clough-Tocher splits have not been used previously in the trivariate setting, and in fact their only appearance in the literature that we are aware of is in [1], where they are used to construct a C^2 bivariate macro-element.

Remark 3. The results here depend critically on the fact that for each tetrahedron $T := \langle v_1, v_2, v_3, v_4 \rangle$, the center v_T and four subcenters v_T^i in the double-Clough-Tocher split of T are chosen as barycenters. In particular, this choice means that for each $i = 1, 2, 3, 4$, the points v_i, v_T, and v_T^i are collinear, where v_T^i is the barycenter of the subtetrahedron in the Clough-Tocher split of T which does not contain v_i. Any perturbation of these points which destroys this geometry would result in a spline space $\mathcal{S}_2(T_{DCT})$ with a different dimension. For example, if all points are in generic position, then the space has dimension 272, but doesn't work as a C^2 macro-element since only 256 of the 264 degrees of freedom needed for global smoothness can be imposed.

Remark 4. C^r trivariate polynomial macro-elements defined on nonsplit tetrahedra were constructed in [14] 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. For $r = 2$, these elements make use of polynomials of degree 17.

Remark 5. C^1 trivariate macro-elements were constructed on the Clough-Tocher split in [2]. For other C^1 trivariate macro-elements, see [18,19].

Remark 6. By examining slices through T_{DCT}, it can be shown that it is not possible to construct C^2 macro-elements on the DCT-split using splines with smoothness less than 4 at the vertices. This in turn implies that the minimal degree possible is nine.

Remark 7. 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. It can be used or downloaded from `http://www.math.utah.edu/~pa/3DMDS`, along with associated documentation. This program computes the dimension of trivariate spline spaces and finds minimal determining sets. This involves analyzing homogeneous linear systems with integer coefficients. The code usually analyzes such systems in residual arithmetic modulo the prime number $P = 2^{31} - 1$, but optionally is also capable of doing the analysis in exact integer arithmetic (at much greater computational expense), which is what we have done here for the proof of Theorem 1. The linear algebra involved in the code is exactly as in the corresponding bivariate code described in [3], and documented in detail at `http://www.math.utah.edu/~pa/MDS`.

Remark 8. Because the smoothness conditions built into the space $\mathcal{S}_2(T_{DCT})$ overlap, a spline s in this space automatically satisfies a number of additional smoothness conditions. In particular,

1) $s \in C^3(e)$ for each of the 4 edges connecting v_T to vertices of T,
2) $s \in C^4(e)$ for each of the 12 edges connecting the v_T^i to vertices of T,
3) $s \in C^7(e)$ for each of the four edges connecting v_T to the v_T^i,
4) $s \in C^3(F)$ for each of the 12 faces of T_{DCT} of the form $\langle v_T^i, v_T, v_j \rangle$, i.e., whose vertices include v_T, one of the v_T^i, and one of the vertices of T.

Remark 9. In analogy with the bivariate case, cf. [4,5], we say that $\mathcal{N}$ is a set of natural degrees of freedom for a macro-element space $\mathcal{S}$ provided it involves only functionals defined at points on the boundary of T which are necessary to ensure the global smoothness. Our space $\mathcal{S}_2(T_{DCT})$ is not defined by a set of natural degrees of freedom because of the derivative data required at the subcenters v_T^i. Clearly, by enforcing an appropriate set of 16 additional special smoothness conditions, it is possible to define a subspace of $\mathcal{S}_2(T_{DCT})$ of dimension 264 with an associated set of natural degrees of freedom. However, we have not been able to find a nice (symmetric) way to describe exactly which 16 conditions will work.

Remark 10. 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 11. 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 [10] for the bivariate case.

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