# A C<sup>2</sup> Trivariate Macro-Element Based on the Worsey-Farin Split of a Tetrahedron

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**Abstract.** A  $C^2$  trivariate macro-element is constructed based on the Worsey-Farin split of a tetrahedron into twelve 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 paper [5] in which we constructed a  $C^2$  trivariate macro-element based on Clough-Tocher splits of a tetrahedron using polynomials of degree thirteen on the subtetrahedra. The purpose of this paper is to describe an alternative  $C^2$  macro-element which works with polynomials of degree nine instead. To be able to use the lower degree polynomials, we have to work with a more complicated split. Here we choose the Worsey-Farin split [23]. It divides a tetrahedron into twelve subtetrahedra, as compared with the four subtetrahedra involved in a Clough-Tocher split.

We recall [5] that a trivariate macro-element defined on a tetrahedron T consists of a pair  $(S, \Lambda)$ , where S is a 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  $s \in S$  with  $\lambda_i s = z_i$  for  $i = 1, \ldots, n$ . These functionals are called the nodal degrees of freedom of the element. 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  $\Delta$ , 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 also give a minimal determining set for the space

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and calculate its dimension. In Sect. 4 we collect several lemmas concerning bivariate spline spaces which are used in our construction. The macro-element space for a Worsey-Farin refinement of an arbitrary tetrahedral partition is discussed in Sect. 5, where again we give a dimension statement and an explicit minimal determining set. Sect. 6 is devoted to the construction of a nodal determining set for our macro-element space, and an associated Hermite interpolation operator along with an error bound for it. We conclude the paper with a number of remarks.

# §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  $\Omega$ , we define

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

In dealing with polynomials and splines, we will make use of well-known Bernstein-Bézier methods as used for example in [1-7,11-24]. 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  $\Delta$  is a tetrahedral partition of a set  $\Omega$ , we write  $\mathcal{D}_{\Delta,d}$  for the collection of all domain points associated with tetrahedra in  $\Delta$ , where common points in neighboring tetrahedra are not repeated. Given  $\xi \in \mathcal{D}_{T,d}$ , we denote the associated Bernstein polynomial by  $B_{\xi}^{T,d}$ .

Given  $\rho > 0$ , we refer to the set  $D_{\rho}(v)$  of all domain points which are within a distance  $\rho$  from v as the ball of radius  $\rho$  around v. Similarly, we refer to the set  $R_{\rho}(v)$  of all domain points which are at a distance  $\rho$  from v as the shell of radius  $\rho$  around v. If e is an edge of  $\Delta$ , we define the tube of radius  $\rho$  around e to be the set of domain points whose distance to e is at most  $\rho$ .

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  $F:=\langle v_1,v_2,v_3\rangle$  is such a face, we write  $\mathcal{D}_{F,d}$  for this set of domain points. As usual, we call the set of points  $D_{\rho}(v_1)$  in  $\mathcal{D}_{F,d}$  within a distance  $\rho$  from  $v_1$  the disk of radius  $\rho$  around  $v_1$ . Similarly, the set of points  $R_{\rho}(v_1)$  in  $\mathcal{D}_{F,d}$  at a distance  $\rho$  from  $v_1$  is called the ring of radius  $\rho$  around  $v_1$ . We use the same notation for disks/balls and shells/rings, but the meaning will be clear from the context.

Suppose  $\mathcal{S}$  is a linear subspace of  $\mathcal{S}_d^0(\Delta)$ , and suppose  $\mathcal{M}$  is a subset of  $\mathcal{D}_{\Delta,d}$ . 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. It is also known that the cardinality of any minimal determining set for  $\mathcal{S}$  equals the dimension of  $\mathcal{S}$ .

Now suppose  $\mathcal{N}$  is a collection of linear functionals  $\lambda$ , where  $\lambda s$  is defined by a combination of values or derivatives of s at a point  $\eta_{\lambda}$  in  $\Omega$ . 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  $v_T$  be a point in the interior of T. In this section we take  $v_T$  to be an arbitrary point in T, but to obtain a  $C^2$  macro-element space on a general tetrahedral partition, we need to be more careful in the selection of the  $v_T$ , see Sect. 5 below. In addition, for each face F of T, let  $v_F$  be a point in the interior of F. For tetrahedral partitions with more than one tetrahedron, we will also have to choose these points in a special way. Suppose now that we connect  $v_T$  to each vertex v of T and to each point  $v_F$ , and we connect each  $v_F$  to the vertices of the face in which it lies. Then T is split into 12 subtetrahedra. This split was used in [23] to construct a  $C^1$  piecewise cubic trivariate macro-element. We refer to it as the Worsey-Farin split and denote it by  $T_{WF}$ . We write  $\mathcal{V}_T$ ,  $\mathcal{E}_T$ , and  $\mathcal{F}_T$  for the sets of vertices, edges, and faces of T. Let  $\mathcal{E}_T^c$  be the set of four edges connecting  $v_T$  to the face points  $v_F$ , and for each  $F:=\langle v_1,v_2,v_3\rangle\in\mathcal{F}_T$ , let  $\mathcal{E}_F$  be the set of three oriented edges  $\langle v_i,v_F\rangle$ , i=1,2,3. We write  $\mathcal{F}_T^0$  for the set of 12 faces of  $\Delta_{WF}$  of the form  $\langle v_T,v_F,v_F\rangle$ , where  $v\in\mathcal{V}_T$ .

We need some additional notation before introducing our basic macro-element. Suppose  $t:=\langle v_T,v_F,v_1,v_2\rangle$  and  $\tilde{t}:=\langle v_T,v_F,v_2,v_3\rangle$  are two tetrahedra in  $T_{WF}$  which share the face  $F:=\langle v_T,v_F,v_2\rangle\in\mathcal{F}_T^0$ . Let  $c_{ijkl}$  and  $\tilde{c}_{ijkl}$  be the coefficients of the B-representations of  $s|_t$  and  $s|_{\tilde{t}}$ , respectively. Then we define the linear functionals  $\nu_F$  and  $\mu_F$  by

$$\nu_F s := \tilde{c}_{0,1,3,5} - \sum_{i+j+k=5} c_{0,i+1,j,k+3} B_{ijk}^{t,5}(v_3), 
\mu_F s := \tilde{c}_{1,0,3,5} - \sum_{i+j+k=5} c_{1,i,j,k+3} B_{ijk}^{t,5}(v_3), \tag{3.1}$$

where  $B_{ijk}^{t,5}$  are the Bernstein polynomials of degree 5 with respect to the triangle  $\langle v_F, v_1, v_2 \rangle$ . Note that  $\nu_F s$  involves coefficients of s on the shell  $R_9(v_T)$ , while  $\mu_F s$  involves coefficients of s on the shell  $R_8(v_T)$ .

We now introduce our basic macro-element space as the following space of

supersplines defined on  $T_{WF}$ :

$$S_{2}(T_{WF}) := \{ s \in C^{2}(T) : s |_{t} \in \mathcal{P}_{9}^{3} \text{ for all } t \in T_{WF},$$

$$s \in C^{3}(e), \text{ for all } e \in \mathcal{E}_{T},$$

$$s \in C^{7}(e), \text{ for all } e \in \mathcal{E}_{T}^{c},$$

$$\nu_{F} s = \mu_{F} s = 0, \text{ for all } F \in \mathcal{F}_{T}^{0},$$

$$s \in C^{4}(v), \text{ for all } v \in \mathcal{V}_{T},$$

$$s \in C^{7}(v_{T}) \}.$$

$$(3.2)_{\text{STWF}}$$

As usual, if v is a vertex of  $T_{WF}$ , 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  $\rho$  at v. If e is an edge of  $T_{WF}$ , 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  $\mu$  on e.

Before proceeding, we first make some remarks about our fairly complicated definition of  $S_2(T_{WF})$ . 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 6. In creating  $S_2(T_{WF})$ , we had two aims in mind: to create a macroelement 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 macroelements on adjoining tetrahedra join with  $C^2$  smoothness, see Remark 4. 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  $S_2(T_{WF})$  has been imposed in order to remove unnecessary degrees of freedom from our macro-element. While other choices are possible, we found that this choice is the most symmetric while at the same time providing stable computations.

For each vertex v of T, let  $T_v$  be one of the tetrahedra in  $T_{WF}$  attached to v. For each edge  $e := \langle u, v \rangle$  of T, let  $T_e$  be one of the two tetrahedra containing e, and let  $E_3(e)$  denote the set of domain points in the tube of radius 3 around e which do not lie in the balls  $D_4(u)$  or  $D_4(v)$ . Finally, for each face  $F := \langle v_1, v_2, v_3 \rangle$  of T, let  $T_{F,i} := \langle v_T, v_F, v_i, v_{i+1} \rangle$ , i = 1, 2, 3, where we set  $v_4 := v_1$ .

WF **Theorem 3.1.** The space  $S_2(T_{WF})$  has dimension 292. Moreover,

$$\mathcal{M} := \bigcup_{v \in \mathcal{V}_T} \mathcal{M}_v \cup \bigcup_{e \in \mathcal{E}_T} \mathcal{M}_e \cup \bigcup_{F \in \mathcal{F}_T} \mathcal{M}_F \cup \mathcal{M}_T$$
(3.3)<sub>WFmds</sub>

is a minimal determining set for  $S_2(T_{WF})$ , where

- 1)  $\mathcal{M}_v := D_4(v) \cap T_v$ ,
- $2) \mathcal{M}_e := E_3(e) \cap T_e,$

3) 
$$\mathcal{M}_F := \{\xi_{2430}^{T_{F,1}}, \xi_{2430}^{T_{F,2}}, \xi_{2430}^{T_{F,3}}\},$$

4) 
$$\mathcal{M}_T := D_3(v_T) \cap T_{v_T}$$
.

**Proof:** We shall show that  $\mathcal{M}$  is a minimal determining set for  $\mathcal{S}_2(T_{WF})$ , which in turn implies that the dimension of  $\mathcal{S}_2(T_{WF})$  is just the cardinality of  $\mathcal{M}$ . The cardinalities of the sets  $\mathcal{M}_v$ ,  $\mathcal{M}_e$ ,  $\mathcal{M}_F$ ,  $\mathcal{M}_T$  are 35, 20, 3, and 20, respectively. Since T has four vertices, six edges, and four faces, it follows that the dimension of  $\mathcal{S}_2(T_{WF})$  is  $4 \times 35 + 6 \times 20 + 4 \times 3 + 20 = 292$ .

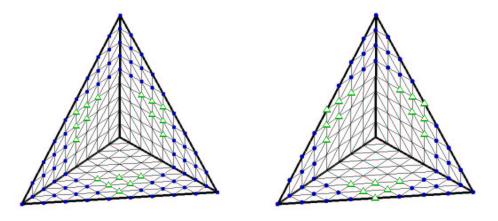
To show that  $\mathcal{M}$  is a minimal determining set for  $\mathcal{S}_2(T_{WF})$ , we need to show that setting the coefficients  $\{c_{\xi}\}_{{\xi}\in\mathcal{M}}$  of a spline  $s\in\mathcal{S}_2(T_{WF})$  uniquely determines all other coefficients of s. First, for each vertex  $v\in\mathcal{V}_T$ , the  $C^4$  smoothness at v implies that all coefficients corresponding to domain points in  $D_4(v)$  are uniquely determined. Moreover, for each edge  $e\in\mathcal{E}_T$ , the  $C^3$  smoothness around e implies that the coefficients of s in the tube of radius 3 around e are uniquely determined.

We now examine the coefficients corresponding to domain points on the shell  $R_9(v_T)$ , i.e., on the outer faces of  $T_{WF}$ . Let  $F := \langle v_1, v_2, v_3 \rangle$  be a face of this shell. We can consider the coefficients of s corresponding to the domain points on F, see Fig. 1 (left), as the coefficients of a bivariate spline  $g := s|_F$  in the space  $\widetilde{S}_9^2(F_{CT})$  defined in (4.2) below, where  $F_{CT}$  is the Clough-Tocher split of F into three subtriangles. By the above, it is clear that all coefficients of g corresponding to the domain points marked with dots or triangles in Fig. 1 (left) are already uniquely determined. But then by Lemma 4.1 below, all other coefficients of g are uniquely determined. Repeating this argument for each face of  $R_9(v_T)$ , we conclude that the coefficients of g are uniquely determined for all domain points on the shell  $R_9(v_T)$ .

Now consider the coefficients of s corresponding to domain points lying on the shell  $R_8(v_T)$ . For each face  $F:=\langle v_1,v_2,v_3\rangle$  of this shell, we can consider the B-coefficients of s corresponding to domain points on F, see Fig. 1 (right), to be the coefficients of a bivariate spline g in the space  $\widetilde{\mathcal{S}}_8^2(F_{CT})$  defined in (4.5) below. It is clear from the above that all coefficients of g corresponding to domain points marked with dots or triangles in Fig. 1 (right) are already uniquely determined. But then by Lemma 4.2 below, all other coefficients of g are uniquely determined. Repeating this argument for each face of  $R_8(v_T)$ , we conclude that the coefficients of g are uniquely determined for all domain points on the shell  $R_8(v_T)$ .

Next we consider the shell  $R_7(v_T)$ . Let F be a face of this shell. We can consider the coefficients of s corresponding to domain points on F to be the coefficients of a bivariate spline g in  $\mathcal{S}_7^2(T_{CT}) \cap C^7(T_{CT})$ , which means that g is actually a polynomial of degree 7. All coefficients corresponding to domain points marked with dots or triangles in Fig. 2 are already uniquely determined. In addition, those corresponding to  $\oplus$  are also uniquely determined as those points are in  $\mathcal{M}$ . It now follows from Lemma 4.3 below that all other coefficients of g are uniquely determined. Repeating this argument for each face of  $R_7(v_T)$ , we conclude that all coefficients of s corresponding to domain points on the shell  $R_7(v_T)$  are uniquely determined.

To show that the coefficients of s corresponding to the remaining domain points



w<sub>F0</sub> Fig. 1. Domain points of  $S_2(T_{WF})$  on faces of  $R_9(v_T)$  and  $R_8(v_T)$ , respectively.

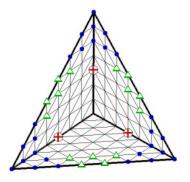


Fig. 2. Domain points of  $S_2(T_{WF})$  on a face of  $R_7(v_T)$ .

WF1

in  $T_{WF}$  are uniquely determined, we note that by the  $C^7$  smoothness at  $v_T$ , we may consider the B-coefficients of s corresponding to domain points in the ball  $D_7(v_T)$  as those of a trivariate polynomial g of degree 7 considered as a spline in  $\mathcal{S}^2_7(t_{WF})$ , where  $t_{WF}$  is the Worsey-Farin split of the tetrahedron t whose vertices are the vertices of  $D_7(v_T)$ . By the above, g is uniquely determined on the faces of t. Now setting the coefficients  $\{c_\xi\}_{\xi\in\mathcal{M}_T}$  is equivalent to setting the derivatives of g up to order 3 at the point  $v_T$ . But then Lemma 3.2 below shows that this combined information uniquely determines g.  $\square$ 

Lemma 3.2. Suppose  $g \in \mathcal{P}_7^3$  and let  $\{c_\xi\}_{\xi \in \mathcal{D}_{t,7}}$  be its set of B-coefficients relative to a tetrahedron t. Suppose we are given values for the coefficients corresponding to the set of domain points lying on the faces of t. Let w be any point in the interior of t. Then the remaining coefficients of g are uniquely determined by the values of  $\{D^{\alpha}g(w)\}_{|\alpha|\leq 3}$ .

**Proof:** The set of domain points in  $\mathcal{D}_{t,7}$  which do not lie on the faces of t is

 $\Gamma := \{\xi_{ijkl}^{t,7} : i,j,k,l \geq 1\}$ . The cardinality of this set is 20. Now the equations

$$D^{\alpha}g(w) = z_{\alpha}, \qquad |\alpha| \le 3,$$

provide a linear system of 20 equations for the  $\{c_{\xi}\}_{\xi\in\Gamma}$ . We claim that this system is nonsingular. To see this, we show that if g is zero on the faces of t and  $z_{\alpha}=0$  for all  $|\alpha|\leq 3$ , then  $g\equiv 0$ . The fact that g vanishes on faces implies that it can be written as  $g=\ell_1\ell_2\ell_3\ell_4q$ , where  $q\in\mathcal{P}_3^3$ , and where for  $i=1,2,3,\,\ell_i$  is a nontrivial linear polynomial which vanishes on the i-th face of t. But now the condition  $D^{\alpha}g(w)=0$  for  $|\alpha|\leq 3$  implies  $D^{\alpha}q(w)=0$  for  $|\alpha|\leq 3$ , which implies  $q\equiv 0$ , which in turn implies that  $g\equiv 0$ .  $\square$ 

#### §4. Some Bivariate Lemmas

In this section we establish some properties of certain bivariate spline spaces defined on the well-known Clough-Tocher split of a triangle  $F := \langle v_1, v_2, v_3 \rangle$  in  $\mathbb{R}^2$ . Given  $v_F$  in the interior of F, we connect it to all three vertices of F to split it into three subtriangles  $F_i := \langle v_F, v_i, v_{i+1} \rangle$ . Let  $e_i := \langle v_i, v_{i+1} \rangle$  and  $\tilde{e}_i := \langle v_i, v_F \rangle$ , i = 1, 2, 3, where  $v_4 := v_1$ . Note that in this section we do not make any special assumptions about the location of  $v_F$ , just that it be in the interior of F. For  $d \geq 2$ , let

$$S_d^2(F_{CT}) := \{ s \in C^2(F) : s|_{F_i} \in \mathcal{P}_d^2, i = 1, 2, 3 \}.$$

Given  $1 \leq l \leq 3$ , suppose  $\{c_{ijk}\}$  and  $\{\tilde{c}_{ijk}\}$  are the coefficients of  $s \in \mathcal{S}_d^2(F_{CT})$  relative to  $F_{l-1}$  and  $F_l$  respectively, where we identify  $v_4 = v_1$ . Then we define the linear functional  $\tau_{l,m,d}^n$  by

$$\tau_{l,m,d}^{n}s := \tilde{c}_{m-n,d-m,n} - \sum_{i+j+k=n} c_{i+m-n,j,k+d-m} B_{ijk}^{l,n}(v_{l+1}), \tag{4.1}_{\text{tau}}$$

where  $B_{ijk}^{l,n}$  are the Bernstein polynomials of degree n relative the triangle  $F_{l-1}$ . Note that  $\tau_{l,m,d}^n$  describes an individual  $C^n$  smoothness condition involving the coefficients on ring  $R_m(v_l)$ .

### ғ9 **Lemma 4.1.** *Let*

$$\widetilde{\mathcal{S}}_{9}^{2}(F_{CT}) := \{ s \in \mathcal{S}_{9}^{2}(F_{CT}) \cap C^{7}(v_{F}) : s \in C^{4}(v_{l}) \\ \text{and } \tau_{l,6,9}^{5}s = 0, \ l = 1, 2, 3 \}.$$

$$(4.2)_{\mathbb{F}^{9}}$$

Then dim  $\widetilde{\mathcal{S}}_{9}^{2}(F_{CT}) = 63$ , and the set

$$\mathcal{M}_9 := igcup_{i=1}^3 ig( \mathcal{M}_{v_i} \cup \mathcal{M}_{e_i} ig)$$

is a minimal determining set for  $\widetilde{\mathcal{S}}_9^2(F_{CT})$ , where

- 1)  $\mathcal{M}_v := D_4(v) \cap t_v$ , where  $t_v$  is some triangle of  $F_{CT}$  attached to v,
- 2)  $\mathcal{M}_e$  is the set of domain points whose distance to  $e := \langle u, v \rangle$  is at most 3, and which do not lie in the disks  $D_4(u)$  or  $D_4(v)$ .

**Proof:** Points in the sets  $\mathcal{M}_e$  are marked with small triangles in Fig. 1 (left), while points in the disks  $D_4(v)$  are marked with dots. By Theorem 2.2 in [19],  $\dim \mathcal{S}_9^2(F_{CT}) \cap C^7(v_F) = 75$ . To get the subspace  $\widetilde{\mathcal{S}}_9^2(F_{CT})$ , for each l = 1, 2, 3 we have to enforce three extra smoothness conditions at the vertex  $v_l$  to get  $C^4(v_l)$  as well as the special smoothness condition corresponding to  $\tau_{l,6,9}^5$ . It follows that  $\dim \mathcal{S}_9^2(F_{CT}) \geq 63$ . Since the cardinality of  $\mathcal{M}_9$  is 63, to show that  $\mathcal{M}_9$  is a minimal determining set for  $\widetilde{\mathcal{S}}_9^2(F_{CT})$  and  $\dim \widetilde{\mathcal{S}}_9^2(F_{CT}) = 63$ , it suffices to show that if s is a spline in  $\widetilde{\mathcal{S}}_9^2(F_{CT})$  whose coefficients satisfy  $c_{\xi} = 0$  for all  $\xi \in \mathcal{M}_9$ , then  $s \equiv 0$ . By the definition of  $\mathcal{M}_9$ , it is clear that all coefficients marked with dots or triangles in Fig. 1 (left) are zero. We now examine the coefficients corresponding to the remaining domain points.

First consider the ring  $R_5(v_1)$ . All coefficients corresponding to domain points on this ring are already zero except for the three corresponding to domain points within a distance 1 of the edge  $\tilde{e}_1$ . To compute these three coefficients, we proceed as in Lemma 3.3 of [9] and Lemma 2.1 of [4]. The  $C^7$  smoothness at  $v_F$  implies that s satisfies individual  $C^1$ ,  $C^2$ , and  $C^3$  continuity conditions on ring  $R_5(v_1)$ , i.e.,  $\tau_{1,5,9}^n s = 0$  for n = 1, 2, 3. This leads to a linear system of equations with matrix

$$M_3 := \begin{pmatrix} a_2 & a_1 & -1 \\ 2a_2a_1 & a_1^2 & 0 \\ 3a_2a_1^2 & a_1^3 & 0 \end{pmatrix}, \tag{4.3}_{\text{M3}}$$

where  $(a_1, a_2, a_3)$  are the barycentric coordinates of  $v_3$  relative to the triangle  $F_1$ . This matrix is nonsingular since its determinant is  $-a_2a_1^4$  and  $a_1, a_2$  are both nonzero. Coefficients on the rings  $R_5(v_2)$  and  $R_5(v_3)$  can be computed in a similar way.

Now consider the ring  $R_6(v_1)$ . At this point, all coefficients corresponding to domain points on the ring  $R_6(v_1)$  are determined to be zero except for the five corresponding to domain points within a distance 2 of  $\tilde{e}_1$ . Now the  $C^7$  smoothness at  $v_F$  implies that s satisfies individual  $C^1$  through  $C^4$  smoothness conditions on ring  $R_6(v_1)$ . Coupling this with the special smoothness condition  $\tau_{1,6,9}^5 s = 0$ , we are led to the system of equations  $\tau_{1,6,9}^n s = 0$  for  $n = 1, \ldots, 5$ . The matrix of this system is

$$M_5 := egin{pmatrix} 0 & a_2 & a_1 & -1 & 0 \ a_2^2 & 2a_2a_1 & a_1^2 & 0 & -1 \ 3a_2^2a_1 & 3a_2a_1^2 & a_1^3 & 0 & 0 \ 6a_2^2a_1^2 & 4a_2a_1^3 & a_1^4 & 0 & 0 \ 10a_2^2a_1^3 & 5a_2a_1^4 & a_1^5 & 0 & 0 \end{pmatrix}.$$
  $(4.4)_{ ext{M5}}$ 

This is a nonsingular matrix since its determinant is equal to  $-a_2^3a_1^9$ . Coefficients on the rings  $R_6(v_2)$  and  $R_6(v_3)$  can be computed in a similar way. Now all remaining coefficients of s can be computed from the smoothness conditions by solving similar nonsingular  $5 \times 5$  systems. We conclude that all coefficients of s must be zero, which completes the proof of the lemma.  $\square$ 

#### F8 **Lemma 4.2.** *Let*

$$\widetilde{\mathcal{S}}_{8}^{2}(F_{CT}) := \{ s \in \mathcal{S}_{8}^{2}(F_{CT}) \cap C^{7}(v_{F}) : s \in C^{3}(v_{l}) \\ \text{and } \tau_{l \, 5 \, 8}^{5} s = 0, \, l = 1, 2, 3 \}.$$

$$(4.5)_{F8}$$

Then dim  $\widetilde{\mathcal{S}}_8^2(F_{CT}) = 48$ , and the set

$$\mathcal{M}_8 := igcup_{i=1}^3 ig( \mathcal{M}_{v_i} \cup \mathcal{M}_{e_i} ig)$$

is a minimal determining set for  $\widetilde{\mathcal{S}}_8^2(F_{CT})$ , where

- 1)  $\mathcal{M}_v := D_3(v) \cap t_v$ , where  $t_v$  is some triangle of  $F_{CT}$  attached to v,
- 2)  $\mathcal{M}_e$  is the set of domain points whose distance to  $e := \langle u, v \rangle$  is at most 2, and which do not lie in the disks  $D_3(u)$  or  $D_3(v)$ .

**Proof:** The proof is very similar to proof of Lemma 4.1, so we can be brief. By Theorem 2.2 in [19],  $\dim \mathcal{S}_8^2(F_{CT}) \cap C^7(v_F) = 54$ . To get the subspace  $\widetilde{\mathcal{S}}_8^2(F_{CT})$ , for each l = 1, 2, 3, we have to enforce one extra smoothness condition at the vertex  $v_l$  to get  $C^3(v_l)$  along with the special smoothness condition corresponding to  $\tau_{l,5,8}^5$ . It follows that  $\dim \widetilde{\mathcal{S}}_8^2(F_{CT}) \geq 48$ . Since the cardinality of  $\mathcal{M}_8$  is 48, to show that it is a minimal determining set for  $\widetilde{\mathcal{S}}_8^2(F_{CT})$  and  $\dim \widetilde{\mathcal{S}}_8^2(F_{CT}) = 48$ , it suffices to show that if  $c_{\xi} = 0$  for all  $\xi \in \mathcal{M}_8$ , then  $s \equiv 0$ . We already know that all coefficients of s corresponding to domain points marked with dots or triangles in Fig. 1 (right) are zero. But then the remaining coefficients can be computed from the same linear systems as in Lemma 4.1.  $\square$ 

#### F7 Lemma 4.3. The set

$$\mathcal{M}_7 := \mathcal{M}_F \, \cap \, igcup_{i=1}^3 ig( \mathcal{M}_{v_i} \cup \mathcal{M}_{e_i} ig)$$

is a minimal determining set for  $\mathcal{P}_7^2 = \mathcal{S}_7^2(T_{WF}) \cap C^7(T_{WF})$ , where

- 1)  $\mathcal{M}_v := D_2(v) \cap t_v$ , where  $t_v$  is some triangle of  $F_{CT}$  attached to v,
- 2)  $\mathcal{M}_e$  is the set of domain points whose distance to  $e := \langle u, v \rangle$  is at most 1, and which do not lie in the disks  $D_2(u)$  or  $D_2(v)$ .

3) 
$$\mathcal{M}_F := \{\xi_{430}^{F_1}, \xi_{430}^{F_2}, \xi_{430}^{F_3}\}.$$

**Proof:** Points in  $\mathcal{M}_F$  are marked with  $\oplus$  in Fig. 2, while points in  $\mathcal{M}_e$  are marked with small triangles. Points in the disks  $D_2(v)$  are marked with dots. The dimension of  $\mathcal{P}_7^2$  is 36 and the cardinality of  $\mathcal{M}$  is also 36. Thus, it suffices to show that  $\mathcal{M}$  is a determining set. Suppose  $s \in \mathcal{P}_7^2$ , and  $c_{\xi} = 0$  for all  $\xi \in \mathcal{M}$ . This means that the B-coefficients of s corresponding to all marked domain points in Fig. 2 (left) are zero. First, we note that the coefficients corresponding to the 3 remaining domain points on  $R_3(v_1)$  can be computed from a nonsingular  $3 \times 3$  linear system with the matrix  $M_3$  given in (4.3). The same holds for the rings  $R_3(v_2)$  and  $R_3(v_3)$ . Now consider  $R_4(v_1)$ . There are 4 unknown coefficients corresponding to the unmarked points on this ring, and they can be computed from a system of 4 equations with matrix

$$M_4 := egin{pmatrix} 0 & a_2 & -1 & 0 \ a_2^2 & 2a_2a_1 & 0 & -1 \ 3a_2^2a_1 & 3a_2a_1^2 & 0 & 0 \ 6a_2^2a_1^2 & 4a_2a_1^3 & 0 & 0 \end{pmatrix}.$$

The determinant of this matrix is  $-6a_1^4a_2^3 \neq 0$ . We can repeat this for the other two vertices  $v_2, v_3$ . The remaining coefficients of s are then determined exactly as in Lemmas 4.1 and 4.2.  $\square$ 

# §5. The Macro-element Space $S_2(\triangle_{WF})$

We now show that the construction of the previous section can be used to define a  $C^2$  macro-element space defined on a general tetrahedral partition, provided that the split points  $v_T$  and  $v_F$  are chosen appropriately. Suppose  $\triangle$  is an arbitrary tetrahedral partition of a polyhedral domain  $\Omega$ , and that the points  $v_T$  are chosen so that for any pair of tetrahedra sharing a common face F, the line connecting the center points passes through the interior of F. This can be insured, for example, by taking  $v_T$  to be the centers of the inscribed balls in each tetrahedron T, see [23]. We now take  $\triangle_{WF}$  to be the refined partition obtained by applying the Worsey-Farin split to each tetrahedron in  $\triangle$ , where for every face F shared by two tetrahedra T and T, the split point  $v_F$  on F is taken to be the intersection of F with the line connecting  $v_T$  and  $v_{\tilde{T}}$ .

Let V,  $\mathcal{E}$ , and  $\mathcal{F}$  be the sets of vertices, edges, and faces of  $\triangle$ , respectively. Let V, E, F be the cardinalities of these sets, and denote the number of tetrahedra in  $\triangle$  by  $N_T$ . We write  $\mathcal{F}^0 = \bigcup_{T \in \triangle} \mathcal{F}^0_T$ , where  $\mathcal{F}^0_T$  is defined in Sect. 3. Let  $\mathcal{E}^c := \bigcup_{T \in \triangle} \mathcal{E}^c_T$ , where  $\mathcal{E}^c_T$  is also defined in Sect. 3. We now define the following macro-element space:

$$S_{2}(\triangle_{WF}) := \{ s \in C^{2}(\Omega) : s|_{t} \in \mathcal{P}_{9}^{3} \text{ all } t \in \triangle_{WF},$$

$$s \in C^{3}(e), \text{ for all } e \in \mathcal{E},$$

$$s \in C^{7}(e), \text{ for all } e \in \mathcal{E}^{c},$$

$$\nu_{F}s = \mu_{F}s = 0, \text{ for all } F \in \mathcal{F}^{0},$$

$$s \in C^{4}(v), \text{ for all } v \in \mathcal{V},$$

$$s \in C^{7}(v_{T}), \text{ for all } T \in \Delta \}.$$

$$(5.1)_{SWF}$$

To define a MDS for  $S_2(\triangle_{WF})$  we need some more notation. For each vertex v of  $\triangle$ , let  $T_v$  be one of the tetrahedra in  $\triangle_{WF}$  attached to v. For each edge  $e := \langle u, v \rangle$  of  $\triangle$ , let  $T_e$  be one of the tetrahedra containing e, and let  $E_3(e)$  denote the set of domain points in the tube of radius 3 around e which do not lie in the balls  $D_4(u)$  or  $D_4(v)$ . Finally, for each face  $F := \langle v_1, v_2, v_3 \rangle$  of  $\triangle$ , let  $T_{F,i} := \langle v_T, v_F, v_i, v_{i+1} \rangle$ , i = 1, 2, 3, where  $v_T$  is the split point of some tetrahedron in  $\triangle$  containing F (if F is a boundary face, there is just one such tetrahedron – otherwise, there are two).

w<sub>Fmds</sub> **Theorem 5.1.** The space  $S_2(\triangle_{WF})$  has dimension  $35V + 20E + 3F + 20N_T$ . Moreover, the set

$$\mathcal{M} := \bigcup_{v \in \mathcal{V}} \mathcal{M}_v \cup \bigcup_{e \in \mathcal{E}} \mathcal{M}_e \cup \bigcup_{F \in \mathcal{F}} \mathcal{M}_F \cup \bigcup_{T \in \Delta} \mathcal{M}_T$$
 (5.2)<sub>wFmds</sub>

is a minimal determining set for  $S_2(\triangle_{WF})$ , where

- 1)  $\mathcal{M}_v := D_4(v) \cap T_v$ ,
- $2) \mathcal{M}_e := E_3(e) \cap T_e,$
- 3)  $\mathcal{M}_F := \{\xi_{2430}^{T_{F,1}}, \xi_{2430}^{T_{F,2}}, \xi_{2430}^{T_{F,3}}\},$
- 4)  $\mathcal{M}_T := D_3(v_T) \cap T_{v_T}$ .

**Proof:** We shall show that  $\mathcal{M}$  is a MDS for  $\mathcal{S}_2(\triangle_{WF})$ . This implies that the dimension of  $\mathcal{S}_2(\triangle_{WF})$  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  $\mathcal{S}_2(T_{WF})$ , we need to show that if  $s \in \mathcal{S}_2(T_{WF})$ , 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  $E_3(e)$  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  $C^3$  smoothness around edges, all other coefficients corresponding to domain points in the sets  $E_3(v)$  will be uniquely determined.

Now we can use Lemma 4.1 to compute coefficients corresponding to the remaining domain points on the faces of the shells  $R_9(v_T)$  for all T. For interior faces

F, this means computing the same coefficients twice, once for each tetrahedron sharing F. But we will get the same values since these coefficients are computed in the same way using only known coefficients associated with domain points on F.

We can now use Lemma 4.2 to uniquely compute coefficients corresponding to the remaining domain points on the faces of the shells  $R_8(v_T)$  for all T. But now we have to check that if  $T:=\langle v_T,v_1,v_2,v_3\rangle$  and  $\widetilde{T}:=\langle v_{\widetilde{T}},v_1,v_2,v_3\rangle$  are two tetrahedra sharing a face  $F:=\langle v_1,v_2,v_3\rangle$ , then these computed coefficients satisfy all  $C^1$  smoothness conditions across F. Note that the split point  $v_F$  lies on the line from  $v_T$  to  $v_{\widetilde{T}}$ . Let  $g:=s|_T$  and  $\widetilde{g}:=s|_{\widetilde{T}}$ . Consider the typical subtriangle  $f:=\langle v_F,v_1,v_2\rangle$  of  $F_{CT}$ . By the geometry, each of the  $C^1$  smoothness conditions involving coefficients associated with domain points in f reduces to a relationship of the form

$$b = sc + rd$$

where (r, s, 0, 0) are the barycentric coordinates of  $v_T$  with respect to the tetrahedron  $\langle v_{\tilde{T}}, v_F, v_1, v_2 \rangle$ . Here b is a coefficient of g corresponding to a domain point  $\xi_b$  in t which lies at a distance 1 from F, i.e., in  $F_8 := R_8(v_T) \cap F$ , see Fig. 1 (right). Similarly, d is a coefficient of  $\tilde{g}$  corresponding to a domain point  $\xi_d$  in  $\tilde{t}$  which lies at a distance 1 from F, i.e., in  $\tilde{F}_8 := R_8(v_{\tilde{T}}) \cap F$ . The coefficient c is a coefficient of g corresponding to the domain point on F which lies on the straight line between  $\xi_b$  and  $\xi_d$ . Let  $\Gamma_8$  be the set of n := 66 domain points in Fig. 1 (right) marked with either a dot or a triangle. Let  $\{b_i\}_{i=1}^n$  and  $\{d_i\}_{i=1}^n$  be the corresponding coefficients of g and  $\tilde{g}$ , respectively, and let  $\{c_i\}_{i=1}^n$  be the coefficients of g corresponding to the associated domain points on F, see Fig. 1 (left). Then by the smoothness of g at vertices and around edges, it is clear that all  $C^1$  continuity conditions with tips at points in  $\Gamma_8$  are satisfied, i.e.,

$$b_i = sc_i + rd_i, \qquad i = 1, \dots, n. \tag{5.3}_{\text{ain}}$$

Now let  $\xi$  be any other domain point in Fig. 1 (right), and let b, c, d be the coefficients entering into the  $C^1$  smoothness condition with a tip at  $\xi$ . Then in view of Lemma 4.2, b can be computed as a linear combination of the  $b_1, \ldots, b_n$ , i.e., there exist  $\{\alpha_i\}_{i=1}^n$  such that

$$b = \sum_{i=1}^{n} \alpha_i b_i. \tag{5.4}_{\text{asum}}$$

Since  $F_8$ , and  $\tilde{F}_8$  are just scaled versions of  $F_9 := F$ , it follows that (5.4) also holds with b's replaced by either c's or d's. But then using (5.3), we have

$$[1, -s, -r] \begin{pmatrix} b \\ c \\ d \end{pmatrix} = [1, -s, -r] \begin{pmatrix} b_1 \cdots b_n \\ c_1 \cdots c_n \\ d_1 \cdots d_n \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = 0,$$

which shows that the  $C^1$  smoothness condition with tip at  $\xi$  and involving b, c, d is also satisfied.

Now for each face of F, we set the coefficients corresponding to  $\mathcal{M}_F$ . These sets are clearly separated from each other, and from the sets  $D_4(v)$  and  $E_3(e)$ . If F is an interior face of  $\triangle$ , then there are two tetrahedra T and  $\tilde{T}$  sharing the face F, and  $\mathcal{M}_F$  lies in just one of them, say T. Next we use the  $C^2$  smoothness conditions to uniquely determine the coefficients for the corresponding points in  $\tilde{T}$ . Now we can use Lemma 4.3 to compute the coefficients of s corresponding to the remaining domain points on faces F of the shells  $R_7(v_T)$  for all T. We now check that these computed coefficients satisfy all  $C^2$  smoothness conditions across F. Each domain point in  $F_7$ , see Fig. 2, is the tip of a  $C^2$  smoothness condition. Assuming a, b, c, d, e are the coefficients on  $F_7$ ,  $F_8$ ,  $F_9$ ,  $\tilde{F}_8$ ,  $\tilde{F}_7$ , the typical condition has the form

$$a = s^2c + 2rsd + r^2e,$$

where r, s are as before. By construction, these smoothness conditions are satisfied for all points  $\xi$  marked with dots, triangles, or  $\oplus$  in Fig. 2. There are n = 45 such points. Writing  $\{a_i, b_i, c_i, d_i, e_i\}_{i=1}^n$  for the associated coefficients, we have

$$a_i = s^2 c_i + 2rsd_i + r^2 e_i, \qquad i = 1, \dots, n.$$

Now if  $\xi$  is any other point in  $F_7$ , then by Lemmas 4.1–4.3, there are  $\alpha_i$  such that

$$[1, -s^2, -2rs, -r^2] \begin{pmatrix} a \\ c \\ d \\ e \end{pmatrix} = [1, -s^2, -2rs, -r^2] \begin{pmatrix} a_1 \cdots a_n \\ c_1 \cdots c_n \\ d_1 \cdots d_n \\ e_1 \cdots e_n \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = 0,$$

which shows that the  $C^2$  smoothness condition with tip at  $\xi$  and involving b, c, d is also satisfied.

To complete the proof, we now apply Lemma 3.2 to uniquely compute the coefficients of s corresponding to the remaining domain points in the balls  $D_7(v_T)$  for all T.  $\square$ 

# §6. 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  $D^{\alpha}$  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  $T \in \Delta$ , 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  $D_e^{\beta}$  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 sets of equally spaced points in the interior of e:

$$\eta_{e,j}^i := \frac{(i-j+1)u + jv}{i+1}, \qquad j = 1, \dots, i,$$
(6.1)<sub>eta</sub>

for all i > 0.

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  $D_{F,i}$  be the directional derivatives associated with the vectors  $\langle v_i, v_F \rangle$  for i = 1, 2, 3, where as before  $v_F$  is the split point in the face F.

If  $\eta$  is a point in  $\mathbb{R}^3$ , we write  $\varepsilon_{\eta}$  for the point-evaluation functional associated with  $\eta$ , so that for any trivariate function,  $\varepsilon_{\eta} f := f(\eta)$ .

nodal Theorem 6.1. The set

$$\mathcal{N} := \bigcup_{v \in \mathcal{V}} \mathcal{N}_v \cup \bigcup_{e \in \mathcal{E}} \mathcal{N}_e \cup \bigcup_{F \in \mathcal{F}} \mathcal{N}_F \cup \bigcup_{T \in \Delta} \mathcal{N}_T$$

$$(6.2)_{\text{WFnodal}}$$

is a nodal minimal determining set for  $S_2(\triangle_{WF})$ , where

1) 
$$\mathcal{N}_v := \{ \varepsilon_v D^{\alpha} \}_{|\alpha| \le 4},$$

2) 
$$\mathcal{N}_e := \bigcup_{i=1}^3 \bigcup_{j=1}^i \{ \varepsilon_{\eta_{e,j}^i} D_e^{\beta} \}_{|\beta|=i},$$

3) 
$$\mathcal{N}_F := \{ \varepsilon_{v_i} D_F^2 D_{F,i}^4 \}_{i=1}^3,$$

4) 
$$\mathcal{N}_T := \{ \varepsilon_{v_T} D^{\alpha} \}_{|\alpha| \leq 3}.$$

**Proof:** It is easy to see that the cardinality of the set  $\mathcal{N}$  matches the dimension of  $\mathcal{S}_2(\triangle_{WF})$  as given in Theorem 5.1. We already know that the set  $\mathcal{M}$  defined in that theorem is a MDS for  $\mathcal{S}_2(\triangle_{WF})$ . Thus, to show that  $\mathcal{N}$  is a NMDS, it suffices to show that if  $s \in \mathcal{S}_2(\triangle_{WF})$ , then setting the values  $\{\lambda s\}_{\lambda \in \mathcal{N}}$  determines all coefficients in the set  $\{c_{\xi}\}_{\xi \in \mathcal{M}}$ .

For each  $v \in \mathcal{V}$ , we can compute the coefficients in  $\mathcal{M}_v$  from the values of the derivatives  $D^{\alpha}s(v)$  corresponding to  $\mathcal{N}_v$ . Then for each edge  $e \in \mathcal{E}$ , the coefficients in  $\mathcal{M}_e$  can be computed from the derivatives of s corresponding to  $\mathcal{N}_e$ . We now use Lemmas 4.1 and 4.2 as in the proof of Theorem 3.1 to compute all remaining coefficients corresponding to domain points on the shells  $R_9(v_T)$  and  $R_8(v_T)$  of tetrahedra in  $\Delta$ .

Now fix  $F \in \mathcal{F}$ , and consider the set  $\mathcal{M}_F$ . It consists of the three domain points  $\{\xi_{2430}^{T_{F,1}}, \xi_{2430}^{T_{F,2}}, \xi_{2430}^{T_{F,3}}\}$ , where  $T_{F,i}$  are three tetrahedra in  $\triangle_{WF}$  lying on one side of F and sharing the face F. These domain points are marked with  $\oplus$  in Fig. 2 (left). To compute the coefficient corresponding to  $\xi_{2430}^{T_{F,1}}$ , we first solve a  $3 \times 3$  system of equations with associated matrix  $M_3$  as in (4.3) to get the coefficients corresponding to the unmarked domain points on  $R_3(v_1)$  in Fig. 2 (left). Then the coefficient corresponding to  $\xi_{2430}^{T_{F,1}}$  can be computed from the value of the derivative  $D_F^2 D_{F,i}^4 s(v_1)$ . The coefficients corresponding to the other two points in  $\mathcal{M}_F$  can be computed in a similar way. Now we can use Lemma 4.3 to compute the coefficients

of s corresponding to the remaining domain points on shells  $R_7(v_T)$ . Finally, as shown in the proof of Theorem 3.1, for each tetrahedron T in  $\triangle$ , we can use the values  $\{\lambda s\}_{\lambda \in \mathcal{N}_T}$  to compute the coefficients  $c_{\xi}$  of s for  $\xi \in \mathcal{M}_T$ .  $\square$ 

Theorem 6.1 shows that for any function  $f \in C^6(\Omega)$ , there is a unique spline  $s \in \mathcal{S}_2(\triangle_{WF})$  solving the Hermite interpolation problem

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

or equivalently,

- 1)  $D^{\alpha}s(v) = D^{\alpha}f(v)$ , for all  $|\alpha| \leq 4$  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  $1 \leq j \leq i$  and  $1 \leq i \leq 3$ , and for all edges e of  $\triangle$ ,
- 3)  $D_F^2 D_{F,i}^4 s(v_i) = D_F^2 D_{F,i}^4 f(\xi), i = 1, 2, 3, \text{ for each face } F := \langle v_1, v_2, v_3 \rangle \text{ of } \triangle,$
- 4)  $D^{\alpha}s(v_{\tau}) = D^{\alpha}f(v_{\tau})$  for all  $|\alpha| \leq 3$  and all tetrahedra  $T \in \Delta$ .

The nodal functionals described in (6.2) involve some derivatives of order higher than 2, even though s is only  $C^2$  globally. However, s is in  $C^4(v)$  at vertices and in  $C^3(e)$  around edges, and so the third and fourth derivatives appearing in  $\mathcal{N}_e$  and  $\mathcal{N}_v$  are well defined. But it is not in  $C^6(v)$  at a vertex v, and so if F is an interior face, then the derivatives in  $\mathcal{N}_F$  are applied to just one of the polynomial pieces of s which share F.

The mapping which takes functions  $f \in C^6(\Omega)$  to this Hermite interpolating spline defines a linear operator  $\mathcal{I}_{WF}: C^6(\Omega) \to \mathcal{S}_2(\triangle_{WF})$ . The construction guarantees that  $\mathcal{I}_{WF}s = s$  for every spline  $s \in \mathcal{S}_2(\triangle_{WF})$ , 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  $\mathcal{S}_2(\triangle_{WF})$ .

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  $\xi$ , the corresponding coefficient  $c_{\xi}$  of s depends only on values of f and its derivatives at points in star(T), where  $T \in \Delta$  is a tetrahedron containing  $\xi$ . Concerning stability, we have

Lemma 6.2. Given a tetrahedral partition  $\triangle$ , let  $\triangle_{WF}$  be a corresponding Worsey-Farin partition, and let  $\theta_{WF}$  be the smallest angle between any two edges in  $\triangle_{WF}$  sharing a vertex. Then

$$|c_{\xi}| \le C \sum_{i=0}^{6} |\Omega_T|^i |f|_{i,\Omega_T},$$

$$(6.3)_{\text{stableWF}}$$

where  $\Omega_T$  is the union of the tetrahedra in star(T), and C is a constant depending only on  $\theta_{WF}$ .

**Proof:** To see that (6.3) holds, we review the computation of the coefficients of s as described in the proof of Theorem 6.1. For domain points in balls of the form  $D_4(v)$ , where v is a vertex of  $\triangle$ , (6.3) follows from the well-known connection between B-coefficients in such a ball and derivatives at v. Then in the next step we compute coefficients in the sets  $\mathcal{M}_e$  from the derivatives corresponding to  $\mathcal{N}_e$ . This involves solving some systems of equations whose stability depends on  $\theta_{WF}$ . Now Lemmas 4.1 and 4.2 are used to compute coefficients corresponding to domain points on shells  $R_9(v_T)$  and  $R_8(v_T)$ . This involves solving linear systems with matrices  $M_3$  and  $M_5$  whose inverses are bounded by a constant depending on  $\theta_{WF}$ . Next we go to the shells  $R_7(v_x)$ . After solving a 3 × 3 systems for the coefficients on the 3-rings around the vertices of a face F of such a shell, we compute the coefficients in  $\mathcal{M}_F$  from the derivatives of s associated with  $\mathcal{N}_F$  (this is where 6th derivatives come in). The bound (6.3) also holds for these coefficients. Now the coefficients corresponding to the remaining coefficients on the shells  $R_7(v_T)$  are computed from Lemma 4.3, which involves solving systems with matrices  $M_4$  and  $M_5$ . Next, we use Lemma 3.2 to solve for the remaining 20 coefficients of  $s|_{D_7(v_m)}$ (written as single polynomial). The matrix  $M_{20}$  of this system depends only on the barycentric coordinates  $(a_1, a_2, a_3, a_4)$  of  $v_{\tau}$ , which are all bounded away from zero by a constant depending on  $\theta_{WF}$ . This insures that the inverse of  $M_{20}$  is also bounded by a constant depending on  $\theta_{WF}$ . These coefficients are then converted to the final coefficients of s on  $D_7(v_T)$  by subdivision about the point  $v_T$ , which is known to be stable.

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

WFerror **Theorem 6.3.** There exists a constant K depending only on  $\theta_{WF}$  such that for every  $f \in C^{m+1}(\Omega)$  with  $5 \le m \le 9$ ,

$$||D^{\alpha}(f - \mathcal{I}_{WF}f)||_{\Omega} \le K|\Delta|^{m+1-|\alpha|}|f|_{m+1,\Omega}, \tag{6.4}$$

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

**Proof:** Since the proof is similar to the proof of Theorem 3.3 in [5] and Theorem 6.2 in [20] (see also [17,18] for similar arguments in the bivariate case), we can be brief. Fix  $T \in \Delta$ , and let  $f \in C^{m+1}(\Omega)$ . Fix  $\alpha$  with  $|\alpha| \leq m$ . By Lemma 4.3.8 of [8], there exists a polynomial  $q := q_{f,T} \in \mathcal{P}_9^3$  such that

$$||D^{\alpha}(f-q)||_{\Omega_T} \le |(f-q)|_{|\alpha|,\Omega_T} \le K_1 |\Omega_T|^{m+1-|\alpha|} |f|_{m+1,\Omega_T}, \tag{6.5}$$

where  $\Omega_T$  is the union of the tetrahedra in  $\operatorname{star}(T)$ . Since  $\mathcal{I}_{WF}p = p$  for all  $p \in \mathcal{P}_9^3$ ,

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

It suffices to estimate the second quantity. Applying the Markov inequality [22] to each of the polynomials  $\mathcal{I}_{WF}(f-q)|_{T_j}$ , where  $T_1, \ldots, T_{12}$  are the tetrahedra in the WF-split of T, we have

$$||D^{\alpha}\mathcal{I}_{WF}(f-q)||_{T_i} \leq K_2|\Delta|^{-|\alpha|}||\mathcal{I}_{WF}(f-q)||_{T_i},$$

where  $K_2$  is a constant depending only on  $\theta_{WF}$ . Let  $c_{\xi}$  be the B-coefficients of the polynomial  $\mathcal{I}_{WF}(f-q)|_{T_j}$  relative to the tetrahedron  $T_j$ . Then combining (6.3) with the fact that the Bernstein basis polynomials form a partition of unity, it is easy to see that

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

Taking the maximum over j and combining this with (6.5) gives

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

which gives

$$||D^{\alpha}(f - \mathcal{I}_{WF}f)||_{T} \le K_{6}|\Delta|^{m+1-|\alpha|}|f|_{m+1,\Omega_{T}}.$$

Finally, we take the maximum over all tetrahedra T in  $\triangle$  to get (6.4).  $\square$ 

# §7. Remarks

- bivariate Remark 1. In the bivariate setting,  $C^r$  macro-elements on various splits have been studied by several authors, see e.g. [3,4,13,14], and references therein.
- trivariate **Remark 2**.  $C^r$  trivariate polynomial macro-elements defined on nonsplit tetrahedra were constructed in [16] 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.
  - c<sub>1</sub> **Remark 3**.  $C^1$  trivariate macro-elements were constructed on the WF-split using splines of degree 3 in [23]. Stability issues and the approximation power were not addressed. For other  $C^1$  trivariate macro-elements, see [1,24].
  - Remark 4. By examining slices through  $T_{WF}$ , it can be shown that it is not possible to construct  $C^2$  macro-elements on the WF-split using splines with smoothness less than 3 around the edges or smoothness 4 at the vertices. This in turn implies that the minimal degree possible is nine.
- Remark 5. In Sect. 5 we have shown that our local construction of a macroelement on a single tetrahedron given in Theorem 3.1 leads to a  $C^2$  macro-element space for general tetrahedral partitions provided for each interior face F, we choose the split point  $v_F$  on F to lie on the line connecting the interior split points  $v_T$  and  $v_{\tilde{T}}$  of the two tetrahedra T and  $\tilde{T}$  which share the face F. This geometry causes the smoothness conditions across F to be essentially univariate in nature. Tests using the java program have shown that without this condition, we do not get  $C^2$  continuity.

- Femark 6. The java code of the first author for examining piecewise polynomial functions on tetrahedral partitions was a key tool in developing the macro-elements described in this paper. The code uses residual arithmetic to compute the dimension of trivariate spline spaces, find minimal determining sets, and solve the smoothness equations. It can be downloaded from http://www.math.utah.edu/~pa/3DMDS, along with associated documentation.
- Remark 7. We have also used the java code to explore the possibility of imposing additional smoothness conditions on our superspline space  $S_2(T_{WF})$  to get a space of dimension 272 which is uniquely determined by the domain points of Theorem 3.1, minus the set  $\mathcal{M}_T$ . 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 that is necessary to ensure the global smoothness and local construction. 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 of the form (4.1). A similar approach was successful in the bivariate case, cf. [3,4] where we used it to get natural degrees of freedom for bivariate macro-element spaces.
- rather than 35 $V + 20E + 9F + 20N_T$ . The corresponding nodal basis (and associated Hermite interpolation operator) requires derivatives up to order 4 only, rather than the order 6 required for the element described here.
- condense **Remark 9**. 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.
  - quasi **Remark 10**. 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 [12] for the bivariate case.
    - Remark 11. Using the java code mentioned in Remark 6, one can easily check that there is a similar  $C^3$  macro element on the WF-split of a tetrahedron which uses splines of degree 13 which are  $C^6$  around the vertices,  $C^5$  around the edges,  $C^9$  at the centroid  $v_T$ , and  $C^9$  along edges connecting  $v_T$  to points  $v_F$ . This space has dimension 984, with 916 natural degrees of freedom, see Remark 7.
    - Lai Remark 12. We have recently learned [10] that Ming-Jun Lai and Alain Le Méhauté have independently studied  $C^r$  macro-elements based on the WF split.

- **Remark 13**. Using the java software, we have also designed  $C^2$  macro-elements based on a trivariate analog of 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 report on this element in [6].
- stable **Remark 14**. It has recently been shown, see [15], that if incenters are used to construct the bivariate Powell-Sabin element, then the stability of the element depends only on the smallest angle in the original triangulation before applying the Powell-Sabin splits. We conjecture that the analogous statement holds here namely, that the stability of our element depends only on the smallest angle in the original tetrahedral partition  $\triangle$  rather than on the smallest angle  $\theta_{WF}$  in  $\triangle_{WF}$ . This is an important distinction, since even though we are using incenters, theoretically the angles in the Clough-Tocher splits of the faces could be arbitrarily small. We are still working on this conjecture.

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#### References

- 1. Alfeld, P., A trivariate Clough-Tocher scheme for tetrahedral data, Comput. Aided Geom. Design 1 (1984), 169–181.
- 2. Alfeld, P., Bivariate splines and minimal determining sets, J. Comput. Appl. Math. **119** (2000), 13–27.
- 3. Alfeld, P. and L. L. Schumaker, Smooth macro-elements based on Powell-Sabin triangle splits, Advances in Comp. Math. **16** (2002), 29–46.
- 4. Alfeld, P. and L. L. Schumaker, Smooth macro-elements based on Clough-Tocher triangle splits, Numer. Math. **90** (2002), 597–616.
- 5. Alfeld, P., and L. L. Schumaker, A  $C^2$  trivariate macro-element based on the Clough-Tocher split of a tetrahedron, submitted.
- 6. Alfeld, P., and L. L. Schumaker, A  $C^2$  trivariate macro-element based on the double Clough-Tocher split of a tetrahedron, submitted.
- 7. Alfeld, P., L.L. Schumaker, and W. Whiteley, The generic dimension of the space of  $C^1$  splines of degree  $d \geq 8$  on tetrahedral decompositions, SIAM J. Numer. Anal. **30(3)** (1993), 889–920.
- 8. Brenner, S. C. and L. R. Scott, *The Mathematical Theory of Finite Element Methods*, Springer-Verlag, New York, 1994.
- 9. Ibrahim, A. and L. L. Schumaker, Super spline spaces of smoothness r and degree  $d \geq 3r + 2$ , Constr. Approx. **7** (1991), 401–423.
- 10. Lai, M. J., private communication.
- 11. Lai, M.-J. and A. LeMéhauté, A new kind of trivariate  $C^1$  spline, Advances in Comp. Math. **21** (2004), 273–292.

- 12. Lai, M.-J. and L. L. Schumaker, On the approximation power of bivariate splines, Advances in Comp. Math. 9 (1998), 251–279.
- 13. Lai, M. J. and L. L. Schumaker, Macro-elements and stable local bases for splines on Clough-Tocher triangulations, Numer. Math. 88 (2001), 105–119.
- 14. Lai, M. J. and L. L. Schumaker, Macro-elements and stable local bases for splines on Powell-Sabin triangulations, Math. Comp. **72** (2003), 335–354.
- 15. Lai, M. J., Schumaker, L. L., Splines on Triangulations, monograph in preparation.
- 16. Le Méhauté, A., Interpolation et approximation par des fonctions polynomiales par morceaux dans  $\mathbb{R}^n$ , dissertation, Univ. Rennes, 1984.
- 17. Nürnberger, G., V. Rayevskaya, L. L. Schumaker, and F. Zeilfelder, Local Lagrange interpolation with  $C^2$  splines of degree seven on triangulations, in Ad-vances in Constructive Approximation, M. Neamtu and E. Saff (eds), Nashboro Press, Brentwood, TN, 2004, 345–370.
- 18. Nürnberger, G., V. Rayevskaya, L. L. Schumaker, and F. Zeilfelder, Local Lagrange interpolation with bivariate splines of arbitrary smoothness, submitted.
- 19. Schumaker, L. L., Dual bases for spline spaces on cells, Comput. Aided Geom. Design 5 (1988), 277–284.
- 20. Schumaker, L. L. and T. Sorokina,  $C^1$  quintic splines on type-4 tetrahedral partitions, Advances in Comp. Math. **21** (2004), 421–444.
- 21. Schumaker, L. L. and T. Sorokina, A trivariate box macro-element, Constr. Approx., to appear.
- 22. Wilhelmsen, D. R., A Markov inequality in several dimensions, J. Approx. Theory 11 (1974), 216–220.
- 23. Worsey, A. J. and G. Farin, An *n*-dimensional Clough-Tocher interpolant, Constr. Approx. **3** (1987), 99–110.
- 24. Worsey, A. J. and B. Piper, A trivariate Powell-Sabin interpolant, Comput. Aided Geom. Design 5 (1988), 177–186.
- 25. Ženišek, Alexander, Polynomial approximation on tetrahedrons in the finite element method, J. Approx. Theory 7 (1973), 334–351.