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Face-to-face partition of 3D space with identical well-centered tetrahedra

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FACE-TO-FACE PARTITION OF 3D SPACE WITH IDENTICAL WELL-CENTERED TETRAHEDRA

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ABSTRACT. The motivation for this paper comes from physical problems defined on bounded smooth domains Ω in 3D. The numerical schemes for these problems are usually defined on some polyhedral domains Ω_h and if there is some additional compactness result available, then the method may converge even if $\Omega_h \to \Omega$ only in the sense of compacts. Hence we use the idea of meshing the whole space and defining the approximative domains as a subset of this partition.

Numerical schemes for which quantities are defined on dual meshes usually require additional quality of the dual mesh. One of the used approaches is the concept of *well-centeredness*, in which the center of circumsphere of any element lies inside that element. We show that one-parametric family of Sommerville tetrahedral elements, whose copies and mirror images tile 3D, build a well-centered face-to-face mesh. Then, shape-optimal value of parameter is computed. For this value of parameter, Sommerville tetrahedron is invariant w.r. to reflection, i.e. 3D space is tiled by copies of a single tetrahedron.

1. INTRODUCTION

One of the widely accepted full models of a compressible, viscous and heat conducting fluid is the Navier-Stokes-Fourier system. For convergence proof to a numerical method for this system in a smooth bounded domain $\Omega \subset \mathbb{R}^3$, developed recently in [2], we are looking for a family of approximative polyhedral domains $\Omega_h, h \to 0$, admitting a mesh $\mathcal{T}_h$ consisting of compact convex tetrahedral elements that have their diameter of the order h, with the following properties.

(M1) The mesh is face-to-face, i.e. any face of any element $K \in \mathcal{T}_h$ is either a subset of $\partial\Omega_h$ or a face of another element $L \in \mathcal{T}_h$.

(M2) The approximative domains Ω_h converge to Ω, in the following sense

$$\Omega \subset \overline{\Omega} \subset \Omega_h \subset \left\{x \in \mathbb{R}^3 | \mathrm{dist}(x, \Omega) < h\right\}. \tag{1}$$

(M3) In every element $K \in \mathcal{T}_h$ there exists a point $x_K \in \mathrm{int}\, K$ such that for K, L sharing a common face σ we have that $x_K x_L$ is orthogonal to σ and

$$d_\sigma := |x_K - x_L| \geq ch > 0, \tag{2}$$

with $c > 0$ a universal constant independent of K and L.

For method developed in [2] we succeeded to relax the condition (2) to $d_\sigma > 0$. Anyway, some works discussed later require the stronger condition (2). Therefore

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we will construct approximative domains and mesh satisfying the conditions (M1-M3) listed above.

Note that the usual convergence $\partial\Omega_h \to \partial\Omega$ in $W^{1,1}$ is substituted by a weaker condition (1) thanks to some additional result on compactness obtained.

The property (M3) emanates from the need of dealing with Neumann boundary condition for the temperature and is introduced by Eymard et al. [1, Definition 3.6]. The easiest way to ensure $d_\sigma > 0$, is to guarantee that the center of a circumsphere (also called circumcenter) of any element building the mesh lies strictly inside that element. This property is called d-well-centeredness, where d denotes the dimension. A special structure of the mesh will then imply also existence of $c > 0$ such that $d_\sigma \geq ch > 0$.

The concept of well-centeredness has been extensively studied by VanderZee et al., see [10] and [11]. However, to our knowledge, there are so far only few applications, moreover without ambitions on rigorous proof of convergence of the method.

Hirani, a coauthor of VanderZee in [10] and [11], with his colleagues uses well-centered elements in [5] for modelling the equations of Darcy's flow model. It describes the flow of a viscous incompressible fluid in a porous medium, with pressure being defined in the circumcenters of the elements. They point out that for *good quality* Delaunay mesh their method works good, and the use of well-centered mesh is therefore not necessary.

Sazonov et al. use well-centered elements in [7] for a co-volume method for the Maxwell's equations. Electric and magnetic fields are defined on mutually orthogonal meshes. As the time step has to be proportional to d_σ, it is necessary to keep it as large as possible. Therefore, well-centered mesh is used. See [7] for details.

In order to satisfy the above requirements for domains Ω_h and their meshes $\mathcal{T}_h$, we construct 3-well-centered face-to-face mesh that covers $\mathbb{R}^3$, whose elements have radius comparable to h. Then for any $\Omega \in C^{0,1}$ given, we simply define Ω_h as a union of elements having non-empty intersection with Ω.

We will mesh the whole 3-dimensional space with an element of one-type and its mirror image. This enables us to compute the exact distance of circumcenters of two neighbouring elements, but it also may reduce both memory demands and computational time.

Obviously, in 2D it is possible to tile the whole space with regular simplices, which are equilateral triangles. In 3D it is not that easy any more, regular tetrahedra cannot tile 3D, see e.g. [8]. However there have been shown many tilings of 3D so far. Sommerville in 1923 [9, p. 56] introduced a one-parameter family of elements that can tile an infinite prism with equilateral-triangular base (see also Goldberg [4]). We will deal with these *Sommerville II type* elements and show the range of the parameter for which they build a 3-well-centered mesh. Such mesh will then fulfil (M1-M3). Moreover, we compute in a sense *ideal value* of the parameter which will guarantee that all the tetrahedra in the mesh are identical.

2. Notation

We work in $\mathbb{E}^3$, a 3-dimensional space endowed with Euclidean coordinates. Then for $m \leq 3$, σ^m or τ^m will denote a simplex, which is a convex hull of $m+1$ affinely independent points in $\mathbb{E}^3$. We recall that points $\{P_0, P_1, \dots, P_m\}$ are affinely independent if

$$\left(\sum_{i=0}^{m} c_i P_i = 0 \quad \& \quad \sum_{i=0}^{m} c_i = 0\right) \Rightarrow c_i = 0,\ \forall i \in \{0, \dots, m\}.$$

Analogously, every simplex σ^m determines an m-dimensional affine space.

We introduce the following list of the used notation.

$A, B, C, \dots$	points in $\mathbb{E}^3$
σ^m, τ^m or also $P_0 P_1 \dots P_m$	m-dimensional simplex
$\mathrm{aff}(\sigma^m)$	affine space determined by (vertices of) σ^m
S_{σ^m}	circumcenter of σ^m
Σ_{σ^m}	incenter of σ^m (center of an inscribed sphere of σ^m)
R_{σ^m}	radius of circumsphere of σ^m
ϱ_{σ^m}	radius of inscribed sphere of σ^m

Note that the above notation can be used independently of the dimension. We will use also the following dimension-dependent notation.

$A = [A^x, A^y, A^z]$	point with its Euclidean coordinates
$\mathbf{n}_{ABC}$	normal vector of the plane ABC
o_{AB}	axial plane of the segment AB
$\mathbf{o}_{AB(C)}$	axis of the segment AB in the plane ABC

3. 3-well-centered mesh of 3-dimensional space

3.1. **Elements.** Following [9], we define tetrahedron $\tau^3(p)$ depending on a positive parameter p with the following Euclidean coordinates of its vertices:

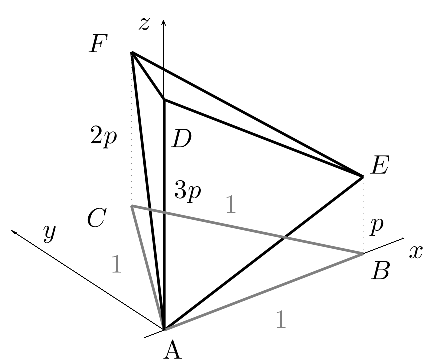

Figure 1. Element $\tau^3(p)$ defined in (3).

$$
\begin{aligned}
&\tau^3(p) := (ADEF)(p), \quad p > 0,\\
&A = [0, 0, 0],\\
&D = [0, 0, 3p],\\
&E = [1, 0, p],\\
&F = \left[\frac{1}{2}, \frac{\sqrt{3}}{2}, 2p\right],
\end{aligned} \tag{3}
$$

see Figure 1. All the vertices and also further derived quantities depend on p, which will be often omitted in the notation for the sake of brevity.

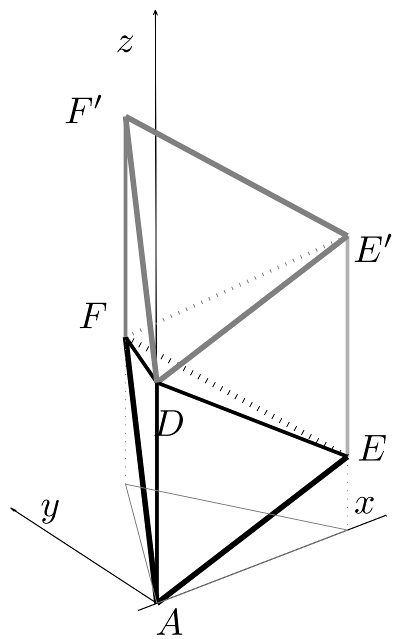

FIGURE 2. Three copies of element $\tau^3(p)$ arranged in a prism with equilateral-triangular base.

3.2. **Tiling the space.** Consider tetrahedra $ADEF(p), DEFE'(p), DE'FF'(p)$, where

$$E' = E + 3p \cdot \overrightarrow{e_3},$$
$$F' = F + 3p \cdot \overrightarrow{e_3},$$

see Figure 2. They are identical and build a skew prism with equilateral triangle as its base. Repeating the structure periodically in the z direction, we can fill the whole infinite prism. It is obvious that with copies and reflections of those prisms we can tile the whole 3-dimensional space, which follows from tiling of 2D with equilateral triangles. The task is to show that we can tile in such way that the elements build a face-to-face mesh.

Lemma 1. *It is possible to create a face-to-face mesh of 3-dimensional space with copies of the tetrahedron $\tau^3(p)$ and its mirror images.*

Proof. After previous discussion it suffices to show that infinite prisms build with elements $\tau^3(p)$ can be arranged such that the elements' edges on the prism surfaces meet. Note that each infinite prism is a convex hull of three vertical lines of three different types, each of them having vertices of elements in the height $3k+r$, $k \in \mathbb{Z}$, for $r = 0, 1, 2$. Projecting the whole situation into xy-plane, it suffices to show that an equilateral triangulation of $\mathbb{E}^2$ is a 3-vertex-colorable graph. As neighbouring triangles in $\mathbb{E}^2$ share an edge, its preimages share a strip where the edges (and thus also the faces) of elements coincide.

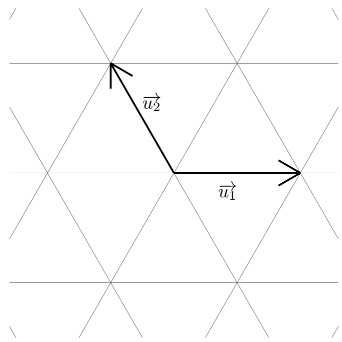

FIGURE 3. Illustration to the proof of Lemma 1: xy-plane with the basis u_1, u_2.

Employing the basis $\overrightarrow{u_1} = (1,0), \overrightarrow{u_2} = \frac{1}{2}\left(-1, \sqrt{3}\right)$, any vertex v of equilateral triangulation of xy plane has unique coordinates, i.e. $\overrightarrow{v} = c_1\overrightarrow{u_1} + c_2\overrightarrow{u_2}$, with *integer values* of c_1, c_2, see Figure 3. Then for vertex v we define its color $\xi(v)$ equal to

$$\xi(v) = c_1 + c_2 \mod 3.$$

Note that for any neighbouring vertices v, w we have

$$\overrightarrow{v} - \overrightarrow{w} = d_1\overrightarrow{u_1} + d_2\overrightarrow{u_2},$$

with $(d_1, d_2) \in \{\,(1,0),\,(1,1),\,(0,1),\,(-1,0),\,(-1,-1),\,(0,1)\,\}$. Hence, we conclude that $\xi(v) \neq \xi(w)$, i.e. ξ is indeed a vertex coloring. □

An alternative proof is suggested in [6]. Reflecting the triplet of elements, shown in Figure 2, with respect to the point $P = (D+E)/2$, we obtain a parallelepiped. Its copies tile the 3-dimensional space and it can be checked that the face-to-face property of the mesh is not violated.

Note that by now, we do not restrict the value of p, i.e. copies and reflections of $\tau^3(p)$ tile $\mathbb{E}^3$ for any $p > 0$.

3.3. **Well-centeredness.** We introduce the concept of well-centeredness by the definition of VanderZee, see [10, p. 5].

Definition 1. Let $0 \le k \le n \le d$. Let $\sigma^n := \{V_0V_1 \dots V_n\}$ be an n-dimensional simplex. A k-dimensional face of σ^n is a simplex $\sigma^k := \{U_0U_1 \dots U_k\}$ with U_i being distinct vertices of σ^n. We say that

(1) σ^n is n-well-centered if its circumcenter lies in the interior of σ^n,
(2) for $1 \le k < n$, σ^n is k-well-centered if all its k-dimensional faces are k-well centered,
(3) σ^n is well-centered if it is k-well centered for all $k \in \{1, \dots, n\}$.

Note that any simplex is 1-well-centered, as the midpoint of any segment lies strictly inside the segment. In $\mathbb{E}^2$, a triangle is well-centered if and only if it is acute.

VanderZee et al. in [10] prove the following characterization for n-well-centeredness of an n-dimensional simplex.

Theorem 2 (VanderZee)**.** *The n-dimensional simplex $\sigma_n = V_0V_1\dots V_n$ is n-well centered if and only if for each $i = 0,\dots,n$ the vertex V_i lies outside circumball $B_i^n := B(V_0, V_1, \dots, V_{i-1}, V_{i+1}, \dots, V_n)$, which is the smallest ball in $\mathbb{E}^n$ which contains the $n-1$ dimensional circumball of the simplex $V_0V_1\dots V_{i-1}V_{i+1}\dots V_n$.*

Theorem 2 will be our tool for proving the following Theorem 3.

Theorem 3. *Tetrahedron $\tau^3(p) = ADEF(p)$ defined by (3) is 3-well-centered if and only if*

$$p < \sqrt{\frac{1}{2}}. \tag{4}$$

Proof. The proof is a simple but laborious computation based on result of Theorem 2, from which we will get the desired restriction on p. The goal is to determine such value of p for which

$$|K - S_{LMN}| > r_{LMN} \tag{5}$$

is valid for all vertices A, D, E, F alternating in the role of K. We have all necessary ingredients for the computation since we can compute

$$S_{LMN} = \mathbf{o}_{LM(N)} \cap \mathbf{o}_{LN(M)}, \tag{6}$$

where

$$\begin{aligned} \mathbf{o}_{LM(N)} &= S_{LM} + t\cdot \mathbf{n}_{LMN} \times \overrightarrow{LM}, \quad t\in\mathbb{R},\\ \mathbf{o}_{LN(M)} &= S_{LN} + t\cdot \mathbf{n}_{LMN} \times \overrightarrow{LN}, \quad t\in\mathbb{R},\\ \mathbf{n}_{LMN} &= \overrightarrow{LM} \times \overrightarrow{LN}, \end{aligned} \tag{7}$$

for given points K, L, M, N.

1. D

   Substituting the ordered quadruplet $[D, A, E, F]$ for $[K, L, M, N]$ in (5), (6), and (7), and performing the computations, we get

$$\begin{aligned} \mathbf{n}_{AEF} &= \left(-\frac{\sqrt{3}}{2}p, -\frac{3}{2}p, \frac{\sqrt{3}}{2}\right),\\ \mathbf{o}_{AE(F)} &= \left[\frac{1}{2}, 0, \frac{p}{2}\right] + u\left(-\frac{3}{2}p^2, \frac{\sqrt{3}}{2}(1+p^2), \frac{3}{2}p\right), \quad u\in\mathbb{R},\\ \mathbf{o}_{AF(E)} &= \left[\frac{1}{4}, \frac{\sqrt{3}}{4}, p\right] + v\left(-\frac{3}{4} - 3p^2, \frac{\sqrt{3}}{4} + \sqrt{3}p^2, 0\right), \quad v\in\mathbb{R}, \end{aligned} \tag{8}$$

   from which we obtain

$$S_{AEF} = \left[\frac{1}{2}(1-p^2), \frac{\sqrt{3}}{6}(1+p^2), p\right].$$

   To conclude for which values of p it holds that $|D - S_{AEF}| > r_{AEF} = |A - S_{AEF}|$, it is sufficient to compare the third component of both expressions only, since A and D differ only in that one. We get

$$|\overrightarrow{e_3} \cdot (S_{AEF} - A)| < |\overrightarrow{e_3} \cdot (S_{AEF} - D)|$$

for any $p > 0$, i.e. condition (5) holds for $K = D, LMN = AEF, p > 0$.

2. F

Using elementary analytic geometry in $\mathbb{E}^2$ (ADE lies in the xz-plane) we obtain the parametric equations of the axes,

$$\mathbf{o}_{AD(E)} = \left[0, 0, \frac{3}{2}p\right] + u(1,0,0), \quad u \in \mathbb{R},$$

$$\mathbf{o}_{AE(D)} = \left[\frac{1}{2}, 0, \frac{1}{2}p\right] + v(p, 0, -1), \quad v \in \mathbb{R},$$

and their intersection

(9) $$S_{ADE} = \left[\frac{1}{2} - p^2, 0, \frac{3}{2}p\right].$$

We want to obtain a bound on p such that

$$|S_{ADE} - F|^2 - r_{ADE}^2 = |S_{ADE} - F|^2 - |S_{ADE} - A|^2 > 0.$$

Substituting from (3), (9) and simplifying we get

(10) $$p < \sqrt{\frac{1}{2}}.$$

3. E

Substituting the quadruplet $[E, A, D, F]$ for $[K, L, M, N]$ into the scheme (5), (6), and (7), one can compute

$$\mathbf{n}_{ADF} = \left(-\frac{3\sqrt{3}}{2}p, \frac{3}{2}p, 0\right),$$

$$\mathbf{o}_{AD(F)} = \left[0, 0, \frac{3}{2}p\right] + u\left(\frac{9}{2}p^2, \frac{9\sqrt{3}}{2}p^2, 0\right), \quad u \in \mathbb{R},$$

$$\mathbf{o}_{AF(D)} = \left[\frac{1}{4}, \frac{\sqrt{3}}{4}, p\right] + v\left(-3p^2, 3\sqrt{3}p^2, -3p\right), \quad v \in \mathbb{R},$$

from which we obtain

(11) $$S_{ADF} = \left[\frac{1}{4} + \frac{1}{2}p^2, \frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{2}p^2, \frac{3}{2}p\right].$$

Again, we want to get bound on p for which

$$|S_{ADF} - E|^2 - r_{ADF}^2 = |S_{ADF} - E|^2 - |S_{ADF} - A|^2 > 0.$$

Substituting from (11), we arrive at

$$p < \sqrt{\frac{2}{3}},$$

which is a weaker requirement than already obtained (10) and therefore does not affect the result.

4. A
   Finally, taking $[K, L, M, N] = [A, D, E, F]$ and performing the computations, we get

$$
\begin{aligned}
&\mathbf{n}_{DEF} = \left(\sqrt{3}p, 0, \frac{\sqrt{3}}{2}\right), \\
&\mathbf{o}_{DE(F)} = \left[\frac{1}{2}, 0, 2p\right] + u\left(0, \frac{\sqrt{3}}{2} + 2\sqrt{3}p^2, 0\right), \quad u \in \mathbb{R}, \\
&\mathbf{o}_{DF(E)} = \left[\frac{1}{4}, \frac{\sqrt{3}}{4}, \frac{5}{2}p\right] + v\left(-\frac{3}{4}, \frac{\sqrt{3}}{4} + \sqrt{3}p^2, \frac{3}{2}p\right), \quad v \in \mathbb{R},
\end{aligned}
\tag{12}
$$

   which gives

$$S_{DEF} = \left[\frac{1}{2}, \frac{\sqrt{3}}{6} - \frac{\sqrt{3}}{3}p^2, 2p\right].$$

   By the same token as in the first case, $|\overrightarrow{e_3} \cdot (S_{DEF} - A)| > |\overrightarrow{e_3} \cdot (S_{DEF} - D)|$ for any value of $p > 0$, which implies that $|A - S_{DEF}| > r_{DEF} = |D - S_{DEF}|$ for any $p > 0$. □

Corollary 4. *Tetrahedron $\tau^3(p)$ is well-centered if and only if*

$$p \in \left(0, \sqrt{\frac{1}{2}}\right).$$

Proof. Using the characterization of an acute triangle (i.e. $a^2 + b^2 > c^2$, where $c \le b \le a$), one can check that for $\tau^3(p), p \in (0, \sqrt{1/2})$ all faces are 2-well-centered. $\tau^3(p)$ is 3-well-centered for $p \in (0, \sqrt{1/2})$ by virtue of Theorem 3. □

VanderZee et al. introduced also a sufficient condition of n-well-centeredness, so called Prism Condition, [11, Proposition 8], which applied to $\tau^{n-1} = AED$ and $v = F$ gives the condition $p < 1/2$. This is more restrictive than the condition (4) which we get by the equivalence criterion in Theorem 2.

We state the following Corollary.

Corollary 5. *Let $\Omega \subset \mathbb{R}^3$ be a smooth (at least Lipschitz) bounded domain. There exists a family of polyhedral domains $\{\Omega_h\}_{h\to 0}$, such that any Ω_h admits a face-to-face mesh $\mathcal{T}_h$, satisfying the conditions (1) and (2).*

Proof. For $h > 0$ and $p \in (0, \sqrt{\frac{1}{2}})$ arbitrary take the tetrahedron $\tau_h^3(p) := \frac{1}{2}h \cdot \tau^3(p)$ and mesh the whole $\mathbb{R}^3$ in the way described in Section 3.2. Denoting the whole mesh with $\tilde{\mathcal{T}}_h$ and defining the set $\mathcal{T}_h := \{K \in \tilde{\mathcal{T}}_h; K \cap \Omega \neq \emptyset\}$, then $\Omega_h := \bigcup_{K \in \mathcal{T}_h} K$.

The face-to-face property follows from Lemma 1. Convergence in the sense of (1) is guaranteed since for $K \in \mathcal{T}_h$ we have

$$\text{diam } \tau_h^3(p) \le \frac{h}{2}\sqrt{1 + (2p)^2} \le h\frac{\sqrt{3}}{2} < h.$$

Finally, the property (2) is satisfied by virtue of Corollary 4 and the fact that the mesh is build by elements with equal radius of inscribed sphere, i.e. $d_\sigma >$

$2\varrho(\tau^3(p))\frac{h}{2}$. The value of $\varrho(\tau^3(p))$ will be specified in the next section, see Proposition 6. ☐

4. Shape optimization

Notice that we have a criterion for the well-centeredness of our elements in a form of an open interval $p \in (0, \sqrt{1/2})$. We would like to get some *optimal value* from the computational point of view, which we expect to be *far enough* especially from the singular value $p = 0$. One of the criteria used (see [3] or [6]) is the so called *normalized shape ratio.* Using the notation introduced in Section 2, we define the normalized shape ratio of tetrahedron σ^3 by

$$\eta(\sigma^3) := \frac{3\varrho(\sigma^3)}{R(\sigma^3)}. \tag{13}$$

The maximal value of (13) is $\eta = 1$ for the regular tetrahedron. In what follows we use shorter notation $\varrho(p) := \varrho(\tau^3(p))$, analogously also for R and η. Next we compute the radii in dependence on p.

Proposition 6. *The radius $\varrho(p)$ of the inscribed sphere of tetrahedron $\tau^3(p)$ equals*

$$\varrho(p) = \frac{3}{4\sqrt{3} + 2\sqrt{4 + \frac{1}{p^2}}}. \tag{14}$$

Proof. Note that having tetrahedron $\tau^3(p)$ placed in Euclidean coordinates, we have $\varrho(p) = \Sigma^y$ where $\Sigma = [\Sigma^x, \Sigma^y, \Sigma^z]$ are the coordinates of the center of the inscribed sphere.

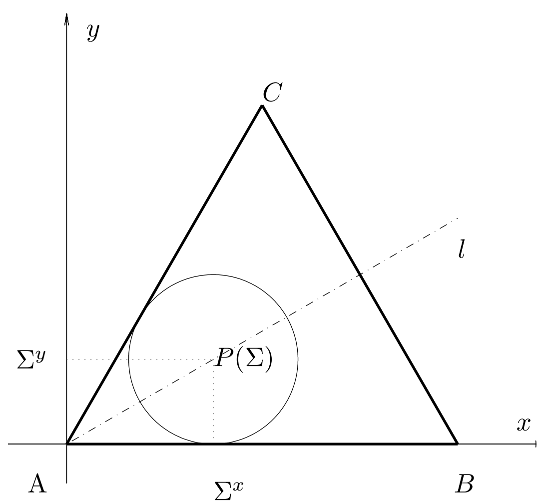

FIGURE 4. Projection of $\tau^3(p)$ and its inscribed sphere into xy-plane.

As the faces ADE and ADF are vertical, orthogonal projection of τ^3 and its inscribed sphere into xy-plane is an equilateral triangle ABC and a circle that touches both segments AB and AC (see Figure 4). The center of the circle $P(\Sigma) = [\Sigma^x, \Sigma^y, 0]$ must lie on a bisector of the $60°$ angle BAC. Hence,

$$\Sigma^x = \sqrt{3}\Sigma^y. \tag{15}$$

Then, the center Σ must lie on α, an axial plane of the dihedral angle of the planes $\operatorname{aff}(AEF)$ and $\operatorname{aff}(DEF)$. Recalling $\mathbf{n}_{AEF}$ and $\mathbf{n}_{DEF}$ from $(8)_1$ and $(12)_1$ respectively, and realizing that their lengths are equal, we can compute

$$\alpha : \quad \mathbf{n}_\alpha \cdot \mathbf{x} + d = 0, \tag{16}$$

with $\mathbf{n}_\alpha = 1/2(\mathbf{n}_{AEF} + \mathbf{n}_{DEF})$. Then d is determined by substituting $\mathbf{x} = E$ into (16) and we get

$$\alpha : \quad \frac{\sqrt{3}}{4}px - \frac{3}{4}py + \frac{\sqrt{3}}{2}z - \frac{3\sqrt{3}}{4}p = 0. \tag{17}$$

Substituting $(\Sigma^x, \Sigma^y, \Sigma^z)$ into (17) and using (15) leads to conclusion that $\Sigma^z = \frac{3}{2}p$. Our problem gets reduced to finding a point

$$\Sigma = \Sigma(p) = \left[\sqrt{3}\varrho(p), \varrho(p), \frac{3}{2}p\right], \tag{18}$$

such that $\operatorname{dist}(AEF, \Sigma(p)) = \varrho(p)$. Such point Σ lies in a plane given by a normal vector $\mathbf{n}_{AEF}$ and point $\varrho(p)\frac{\mathbf{n}_{AEF}}{|\mathbf{n}_{AEF}|}$. The general equation of this plane can be expressed as

$$\mathbf{n}_{AEF} \cdot (x, y, z)^T - \varrho(p)\frac{|\mathbf{n}_{AEF}|^2}{|\mathbf{n}_{AEF}|} = 0,$$

which is

$$-\frac{\sqrt{3}}{2}px - \frac{3}{2}py + \frac{\sqrt{3}}{2}z - \varrho(p)\sqrt{3p^2 + \frac{3}{4}} = 0. \tag{19}$$

Substituting (18) to (19) yields the final result. □

Proposition 7. *The radius of the circumsphere to tetrahedron $\tau^3(p)$ is given by*

$$R(p) = \sqrt{\frac{4}{3}p^4 + \frac{11}{12}p^2 + \frac{1}{3}}. \tag{20}$$

Proof. For the radius we have that $R = |S - A| = |S|$. Hence only the center $S = [S^x, S^y, S^z]$ of circumsphere is of our interest. We proceed in two steps. Firstly, $|SD| = |SA| = |SE|$ suffices to determine both S^x and S^z. The point S must lie on a line which is a cross-section of axial planes o_{AE} and o_{DE},

$$o_{AE} : \left[\frac{1}{2}, 0, \frac{p}{2}\right] + r(0,1,0) + s(-p,0,1), \quad r, s \in \mathbb{R},$$
$$o_{DE} : \left[\frac{1}{2}, 0, 2p\right] + r(0,1,0) + t(-2p,0,-1), \quad r, t \in \mathbb{R}.$$

From this we easily conclude that

$$S \in (o_{AE} \cap o_{DE}) = (S^x, 0, S^z) + r(0,1,0), \quad r \in \mathbb{R}, \tag{21}$$

where further computation gives $S^x = \frac{1}{2} - p^2$ and $S^z = \frac{3}{2}p$.

In the second step we determine S^y by computing the appropriate value of parameter r in (21) from the equality $|SA| = |SF|$, we get

$$S = \left[\frac{1}{2} - p^2, \frac{1}{\sqrt{3}}\left(\frac{1}{2} - p^2\right), \frac{3}{2}p\right].$$

We finish the proof with computing $R = |S|$, which gives (20). □

Theorem 8. *Let $\tau^3(p), p \in (0, \sqrt{1/2})$ be a one-parameter family of tetrahedra defined in (3). Let $\varrho(p)$ be the radius of its inscribed sphere and $R(p)$ radius of its circumsphere. Then $\eta(p)$ defined by (13) is maximal for*

$$p = p^\star = \sqrt{\frac{1}{8}}.$$

Proof. Both $\varrho(p), R(p)$ being continuously differentiable, one can search for the optimum as a point of vanishing derivative. If we obtain one critical point in $\mathbb{R}^+$, it has to be maximum since $\eta(p) > 0$ and

$$\lim_{p\to 0^+} \eta(p) = \lim_{p\to\infty} \eta(p) = 0. \tag{22}$$

The relations in (22) are derived using basic algebra of limits from

$$\lim_{p\to 0^+} \varrho(p) = 0, \qquad \lim_{p\to 0^+} R(p) = \frac{\sqrt{3}}{3},$$

and

$$\varrho(p) < 1, \text{ for all } p > 0, \qquad \lim_{p\to\infty} R(p) = \infty.$$

Solving $\eta'(p) = 0$, leads to searching for roots of

$$32\left(2 + \sqrt{3}\cdot\sqrt{\frac{1}{p^2} + 4}\right)p^6 + \left(30 + 11\sqrt{3}\cdot\sqrt{\frac{1}{p^2} + 4}\right)p^4 - 2 = 0,$$

which, employing new variable $b = p^2$, can be shown to have unique solution in positive real half-axis which is $b^\star = 1/8$, therefore $p^\star = \sqrt{1/8}$. □

Note that $\tau^3(p^\star)$ is unique in the family of Sommerville II type tetrahedra having the property that it is identical with its mirror image. Therefore, for $p = p^\star$, we get a mesh that is build by copies of a single element. Moreover, $\tau^3(p^\star)$ has all faces identical—isosceles triangles with the ratio of the leg to the base equal to $\sqrt{3}/2$. Dihedral angles of $\tau(p^\star)$ are equal to 90° at the longer edges and 60° at the shorter ones. Naylor in [6] calls $\tau(p^\star)$ an *isotet*, or it is called simply the *Sommerville tetrahedron*. Substituting $p^\star$ into (14) and (20) gives

$$\eta(p^\star) = \frac{3\varrho(p^\star)}{R(p^\star)} = \sqrt{\frac{9}{10}} \approx 0.949.$$

As for Naylor, (see [6]), this is a maximal value of η for meshing 3-dimensional space with a single element type.

Remark 1. *Analogously, it can be shown that the value $p = p^\star$ is ideal also is the sense of maximizing the ratio of inscribed sphere to the diameter of an element. Note that* $\operatorname{diam}\, \tau^3(p) = \sqrt{1+4p^2}$. *One can compute that*

$$\kappa(\tau^3(p^\star)) := \frac{\varrho(p^\star)}{\operatorname{diam}\, \tau^3(p^\star)} = \frac{\frac{\sqrt{3}}{8}}{\sqrt{\frac{3}{2}}} = \frac{\sqrt{2}}{8}.$$

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