Optimization of Subdivision Invariant Tetrahedra

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While two-dimensional triangles are always subdivision invariant, the same does not always hold for their three-dimensional counterparts. We consider several interesting properties of those three-dimensional tetrahedra that are subdivision invariant and offer them a new classification. Moreover, we study the optimization of these tetrahedra, arguing that the second Sommerville tetrahedra are the closest to being regular and are optimal by many measures. Anisotropic subdivision invariant tetrahedra with high aspect ratios are characterized. Potential implications and applications of our findings are also discussed.

Keywords: Subdivision invariant tetrahedron and Second Sommerville tetrahedron and Centroidal Voronoi Tessellation and Optimal triangulation and Optimal tetrahedron and Regular tetrahedron and Unstructured mesh generation and optimization

1. Introduction

This work is mainly concerned with three-dimensional subdivision invariant tetrahedra. Here, subdivision refers to a special operation of a tetrahedron that introduces six new vertices at the midpoints of edges and connects the midpoints of the adjacent edges and one additional pair of opposing midpoints to form a simplicial complex with 8 smaller tetrahedra [7,23,27]. This operation is called a red refinement in adaptive finite element literature [37,40] or a subdivision by Freudenthal's algorithm [26]. A number of works [8,23,40] discuss the number of congruence classes generated by the Freudenthal's algorithm (red refinement). Congruence is defined as follows [8]: two simplices T, T' are called congruent to each other if there exists a translation vector v, a scaling factor c, and an orthogonal matrix Q such that $T' = v + cQT$. In some recent studies, a more restrictive notion of congruence, namely proper con-

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gruence that requires the orientation order to be preserved, has been adopted [37]. We make no such restriction here. Subdivision invariant tetrahedra, abbreviated as SITet (representing both singular and plural forms), are those tetrahedra whose subdivided tetrahedra (using red refinement or Freudenthal's algorithm) contain only a unique congruence class [27,28,47]. In other words, to be a SITet, the eight smaller tetrahedra created by the subdivision must all be congruent, after a scaling, to the original one.

There are various problems that motivate our study of SITet, ranging from the theoretical quests of three-dimensional tiling and packing of geometric objects to practical applications of three-dimensional tetrahedral mesh generation and optimization. For example, simplicial meshing is a popular tool in scientific simulations and engineering design [4,22,42]. It is widely accepted that triangular meshing in two space dimensions has become a relatively mature subject, and the theory of which is well understood. In contrast, the progress towards an automated and optimized meshing technology has been slow for three- or higher-dimensional simplicial meshing. On the one hand, this can be attributed to the enormous complexities associated with the transient and adaptive nature of large-scale physical systems and complex geometric environment. On the other hand, this is also due to the lack of fundamental understanding of some of the basic theoretical questions concerning space subdivisions in high-dimension. Several long-standing conjectures on the mathematics of space-tiling and packing, such as the 3D Kepler conjecture, were solved only in the last decade, while many important questions remain open [13,33,38]. Similarly, for optimal simplicial meshing, while the optimal two-dimensional triangle is typically associated with the regular triangle, the answer becomes unclear in three dimensions as regular tetrahedra fail to be space-filling. Studies in [14] suggest that regular tetrahedra may not be able to pack as densely as spheres in three dimensional space. Indeed, a gap with dihedral angle $2\pi - 5\theta = 7°21'$ is left unfilled when five identical regular tetrahedra are glued together around a common edge. This is a simple fact, but several renowned scholars have made mistakes regarding packings of regular tetrahedra, and many questions about these packings remain unsolved [38]. The earliest and perhaps also the most famous mistake has been attributed to Aristole [3] and created a controversy that lasted for nearly 2000 years. The mystery surrounding this kind of puzzle has also partly contributed to the study of Hilbert's 18th problem [34].

Concerning space-tiling tetrahedra, the first systematic study is believed to have been given by Sommerville [48] in the early twentieth century. The issue of classifying tetrahedra that can tile three-dimensional Euclidean space was raised. It has been stated as an open problem to determine those shapes of tetrahedra whose properly congruent (that is, congruent by an orientation-preserving isometry) copies tile the entire space [38,47]. A related study was carried out in [31]. A recent result was given in [25] showing that in the proper (orientation-preserving) and face-to-face context there are only four tetrahedral tilers up to similarity, verifying the original claims

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of Sommerville. The problem remains open if mirror reflections are allowed.

Subdivision invariant tetrahedra form a subclass of space-filling tetrahedra. Subdivision invariance provides many additional nice features that are useful in geometrical modeling and mesh generation, especially when it is desirable to produce multilevel meshes or to perform local mesh refinement to enhance geometric resolution and simulation/solver efficiency. Obviously, if proper congruence is required, then by [48] and [25], only a finite number of congruent tetrahedral shapes can possibly be subdivision invariant. In fact, a recent study in [37] showed that only one congruent class of such tetrahedra exists. Without requiring orientation consistency, it has been shown in [27,28] that there are possibly four types of such tetrahedra, each type containing infinite number of congruent classes parametrized by a single variable. Our study here further demonstrates that the four types are in fact equivalent, so that effectively there exists a unique type of SITet that can be parametrized by a single scalar variable. This gives our first main result. We also provide additional features of these SITet, such as certain universal relations between the edges, dihedral angles, and faces, that have not been presented before.

In tetrahedra based geometric modeling and tetrahedral mesh generation, mesh optimization is often carried out together with the domain triangulation. The notion of mesh optimality has remained a subject worthy of careful examinations. For isotropic tetrahedral meshes, forcing all tetrahedra into equal-sized regular tetrahedra might be desirable but is impossible to achieve since regular tetrahedra are not space-filling. Unfortunately, it has been a common and popular practice in three dimensional unstructured tetrahedral meshing to take the regular tetrahedron as the ideal element. While such a practice may make most tetrahedra close to being regular, due to the low packing density of regular tetrahedra [14], it is inevitable that sliver elements are often produced to fill in the gaps left in between. Sophisticated techniques developed in the meshing community are then needed for effective sliver removal [12,24,46,49]. This is a scenario that can be perhaps characterized as the intrinsic geometric frustration in three dimensional triangulation, a phenomenon that also reflects a larger issue concerning the proper extensions of two (or lower) dimensional mathematical concepts to three (or higher) dimensions. While many similarities and common features can be documented, there are sometimes fundamental differences in geometric notions when the dimension changes. As an illustration, we advocate the notion of optimal or ideal tetrahedra to be restricted to tetrahedra the class of space-filling tetrahedra or in particular the class of subdivision invariant tetrahedra. This is completely consistent with the conventional (unrestricted) definition in two dimension, but it has dramatically different implications in three and higher dimensions. A natural question is to identify such optimal tetrahedra, upon specification of a suitable metric of optimality, via optimization over all space-filling or subdivision invariant tetrahedra.

Since SITet form an important subclass of space-filling tetrahedra and possess extra nice properties in mesh generation, and because SITet have been completely classified in three dimension already, we make the second important contribution

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of this work by exploring optimization of SITet with respect to various metrics. An interesting finding is that while many different metrics are taken, all aimed at making the tetrahedron more symmetric or regular, the optimal tetrahedron under those metrics are all given by a unique tetrahedron, namely, the second Sommerville tetrahedron. This finding is consistent with studies of other optimization problems concerning space tessellations, in particular, the so-called centroidal Voronoi tessellations. We are thus led to further discussions on how our findings may impact the subject of Voronoi tessellations and Delaunay triangulations as well as three-dimensional tetrahedral mesh generation and optimization. In fact, three-dimensional mesh optimizations of unstructured tetrahedral meshes based on the centroidal Voronoi tessellations have often led to the spontaneous appearance of large patches of second Sommerville tetrahedra [20]. Computational studies of space filling tetrahedra given in [41] also led to the second Sommerville tetrahedra based on various measures. Moreover, numerical solutions of partial differential equations based on such meshes also offer nice superconvergent properties that are generally associated with structured meshes [11]. It is thus no coincidence that while much of the discussion here is elementary, our findings should have far-reaching implications.

The rest of this paper is organized as follows: we first discuss the SITet and the special second Sommerville tetrahedron (SSTet) through some geometric illustrations in section 2, along with a classification of SITet; we then study a number of properties of SITet in section 3; section 4 is devoted to optimizations of SITet and finally some conclusions are given in section 5.

2. Subdivision invariant tetrahedra

The subdivision considered here refers to only bisection or red refinement.

Definition 1. A *subdivision invariant* tetrahedron can be divided into eight tetrahedra that are congruent, with possible mirror-reflections and a scaling, to the original tetrahedron.

2.1. *Subdivision into tetrahedra: some examples*

We begin our discussion of SITet with a couple of examples that also serve to offer some geometric intuition.

Among the most widely studied SITet are those obtained by subdividing a unit cube into six congruent tetrahedra [38]. Let u_1 and u_2 be two opposing vertices on a diagonal of the unit cube, and $\{v_i\}_{i=1}^6$ be the other six vertices of the cube so that $\{v_iv_{i+1}\}$ (with $v_7 = v_1$) gives a directed loop made of six edges of the cube. Then, the six tetrahedra having vertices $\{u_1u_2v_iv_{i+1}\}$ form a congruent tetrahedron packing of the unit cube. Since unit cubes tile the space nicely, we thus obtain a tetrahedron tiling of space. The tetrahedra involved in the tiling have edge ratios $1 : 1 : 1 : \sqrt{2} : \sqrt{2} : \sqrt{3}$, in contrast to regular tetrahedra that have all edges of the same length.

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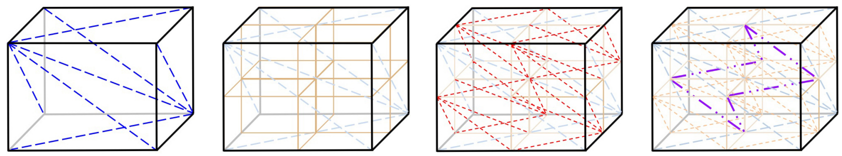

Fig. 1. Invariant subdivision of a cubic domain.

Another very popular class of SITet is given by the second Sommerville tetrahedron, which we will abbreviate as SSTet. It can also be constructed using unit cubes or the BCC lattice: one simply takes two neighboring unit cubes and connects the centers of two cubes with a particular pair of vertices of their shared edges, as shown in Figure 2. SSTet again tile the whole three dimensional space, but not a single unit cube. The SSTet have edge ratios $1:1:1:1:2\sqrt{3}/3:2\sqrt{3}/3$.

Comparing the above two examples of SITet, we see firstly that SITet may not have a unique shape, and secondly, that the edge ratios of SSTet are closer to 1 than those of the other example, thus making the SSTet the closer of the two to being a regular tetrahedra in some sense. More discussions and clarifications are to be given later along these directions.

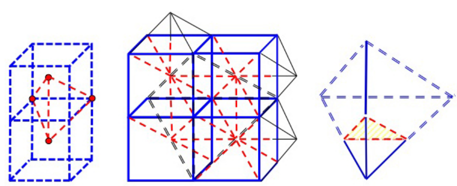

Fig. 2. Construction of subdivision invariant second Somerville tetrahedra.

2.2. *Classification of subdivision invariant tetrahedra*

To classify all SITet, we consider a typical tetrahedron represented by vertices $p_1p_2p_3p_4$. Upon translation and rotation, without loss of generality, we may set p_1 at the origin, p_2 on the positive x-axis with unit distance to p_1, p_3 in the first quadrant on the xy-plane, and p_4 in the first octant of xyz-space. With this set-up, the following result has been provided in [27].

Lemma 1. *(Fuchs [27]) A tetrahedron (as shown in Figure 3) with vertices*

$$p_1 = 0,\ p_2 = \begin{pmatrix}1\\0\\0\end{pmatrix},\ p_3 = \begin{pmatrix}x_1\\y_1\\0\end{pmatrix},\ p_4 = \begin{pmatrix}x_2\\y_2\\z\end{pmatrix}, \quad (\,x_1, x_2, y_2 \geq 0,\ y_1, z > 0\,)$$

is subdivision invariant iff one of the following conditions is fulfilled:

Condition 1: $\quad 0 \leq x_1 < \frac{1}{2}, \quad x_2 = 2x_1, \qquad y_1^2 = 1 - x_1^2,$

$$y_2^2 = \frac{(1+x_1)(1-2x_1)^2}{1-x_1}, \quad z^2 = \frac{(1+x_1)(1-2x_1)}{1-x_1}.$$

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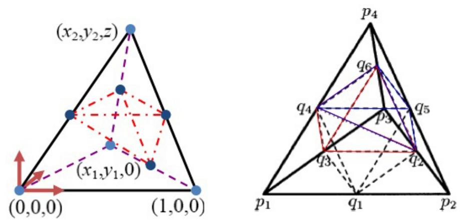

Fig. 3. Subdivision invariant tetrahedra.

Condition 2: $y_2 > 0, \quad x_1 = \dfrac{1}{3}, \quad x_2 = \dfrac{2}{3}, \quad y_1 = 2y_2, \quad z = \sqrt{3}y_2.$

Condition 3: $0 \le x_1 < \dfrac{1}{2}, \quad x_2 = 1 - x_1, \quad y_1^2 = 1 - x_1^2,$

$$y_2^2 = \frac{x_1^2(1+x_1)}{1-x_1}, \quad z^2 = \frac{(1+x_1)(1-2x_1)}{1-x_1}.$$

Condition 4: $0 < x_1 < 3, \quad x_2 = \dfrac{1}{2}(x_1+1), \quad y_1^2 = x_1(3-x_1),$

$$y_2^2 = \frac{1}{4}x_1(3-x_1), \quad z^2 = \frac{1}{4}(3-x_1).$$

We note that each of the conditions is parametrized by a single control variable: x_1 for conditions 1, 3, and 4; and y_2 for condition 2. Given a condition and an input value of the control variable (x_1 or y_2) within the specified bounds, we can determine the remaining vertices.

Remark 1. We note that while we have assumed that all vertices are in the first octant, the tetrahedra generated by the conditions 1 and 3 in Lemma 1 can be constructed as long as $-1 < x_1 < 1/2$.

3. Properties of subdivision invariant tetrahedra

We first consider the edges of SITet. Let points A, B, C, and D refer to vertices p_1, p_2, p_3, and p_4 as defined in Lemma 1. Direct calculations of edge lengths are given below.

Condition 1:

$$\begin{aligned}
AB &= \sqrt{1^2+0^2+0^2} &&= 1,\\
BC &= \sqrt{(x_1-1)^2+y_1^2+0^2} &&= \sqrt{2-2x_1},\\
CD &= \sqrt{(x_2-x_1)^2+(y_2-y_1)^2+z^2} &&= 1,\\
AC &= \sqrt{x_1^2+y_1^2+0^2} &&= 1,\\
AD &= \sqrt{x_2^2+y_2^2+z^2} &&= \sqrt{2-2x_1},\\
BD &= \sqrt{(x_2-1)^2+y_2^2+z^2} &&= \sqrt{3-6x_1}.
\end{aligned}$$

With $0 \le x_1 < 1/2$, we have $AB = CD = AC = 1 \le BC = AD$.

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Condition 2:

$$\begin{aligned}
AB &= \sqrt{1^2+0^2+0^2} &&= 1,\\
BC &= \sqrt{(x_1-1)^2+y_1^2+0^2} &&= \frac{\sqrt{36y_2^2+4}}{3},\\
CD &= \sqrt{(x_2-x_1)^2+(y_2-y_1)^2+z^2} &&= \frac{\sqrt{36y_2^2+1}}{3},\\
AC &= \sqrt{x_1^2+y_1^2+0^2} &&= \frac{\sqrt{36y_2^2+1}}{3},\\
AD &= \sqrt{x_2^2+y_2^2+z^2} &&= \frac{\sqrt{36y_2^2+4}}{3},\\
BD &= \sqrt{(x_2-1)^2+y_2^2+z^2} &&= \frac{\sqrt{36y_2^2+1}}{3}.
\end{aligned}$$

With $y_2 > 0$, we get $CD = AC = BD \leq BC = AD$, and $AB = 1$.

Condition 3:

$$\begin{aligned}
AB &= \sqrt{1^2+0^2+0^2} &&= 1,\\
BC &= \sqrt{(x_1-1)^2+y_1^2+0^2} &&= \sqrt{2-2x_1},\\
CD &= \sqrt{(x_2-x_1)^2+(y_2-y_1)^2+z^2} &&= \sqrt{3-6x_1},\\
AC &= \sqrt{x_1^2+y_1^2+0^2} &&= 1,\\
AD &= \sqrt{x_2^2+y_2^2+z^2} &&= \sqrt{2-2x_1},\\
BD &= \sqrt{(x_2-1)^2+y_2^2+z^2} &&= 1.
\end{aligned}$$

With $0 < x_1 < 1/2$, we get $AB = AC = BD = 1 \leq BC = AD$.

Condition 4:

$$\begin{aligned}
AB &= \sqrt{1^2+0^2+0^2} &&= 1,\\
BC &= \sqrt{(x_1-1)^2+y_1^2+0^2} &&= \sqrt{x_1+1},\\
CD &= \sqrt{(x_2-x_1)^2+(y_2-y_1)^2+z^2} &&= 1,\\
AC &= \sqrt{x_1^2+y_1^2+0^2} &&= \sqrt{3x_1},\\
AD &= \sqrt{x_2^2+y_2^2+z^2} &&= \sqrt{x_1+1},\\
BD &= \sqrt{(x_2-1)^2+y_2^2+z^2} &&= 1.
\end{aligned}$$

With $0 < x_1 < 3$, we have $AB = CD = BD = 1 \leq BC = AD$.

Based on direct calculations of the edge lengths, it becomes trivial to check the subdivision invariance of the tetrahedra specified in Lemma 1. For example, with condition 2, one may check that the length of the two opposing mid-points q_2 and q_4 as shown in Figure 3 is given by $|q_2q_4| = \sqrt{y_2^2+1/9}$, which is precisely

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half of $BC = AD$. This leads to the congruence of all eight subdivided tetrahedra. Moreover, we have the following result.

Lemma 2. *A SITet has at least two pairs of equal opposing edges. More specifically, it has three edges of equal lengths with a pair of them being opposing edges, an additional pair of opposing edges of equal lengths that are longer, and a single edge of a possibly different length.*

Proof. This follows from the direct calculation of edge lengths. □

For easy reference, we call the three edges with equal lengths type-III edges, the two longer edges type-II edges, and the remaining edge a type-I edge. As noted in later discussions, the length of the type-I edge becomes the same as the length of the type-III edges only for the SSTet.

We now present one of our main findings. It shows that the tetrahedra classified by the four conditions given in the Lemma 1 above are in fact determined by a single class through similarity transforms.

Theorem 1. *Tetrahedra generated by one of the four conditions in Lemma 1 are similar to those generated by any of the other conditions.*

Proof. Conditions 1 and 3 obviously generate similar tetrahedra with an interchange of vertices B and C.

As for the other cases, we first look at the edge lengths produced by different conditions. For the statement in the theorem to be true, the ratios of lengths of edges of different types must be the same for some input in different conditions. Let us start with condition 1 and condition 2. For clarity, let us denote the x_1 in condition 1 c_1 and the y_2 in condition 2 c_2. The three ratios are

$$\sqrt{3-6c_1} : 1, \quad 3 : \sqrt{36c_2^2+1}, \quad 3\sqrt{2-2c_1} : \sqrt{36c_2^2+4}.$$

By setting the first two equal to each other, we get a relation $2c_1 = 1-3/(36c_2^2+1)$. Using this, we get all three ratios identical since $2-2c_1 = (36c_2^2+4)/(36c_2^2+1)$.

Similarly, by comparing ratios given by condition 1 with $x_1 = c_1$ and condition 4 with $x_1 = c_4$, we get that $\sqrt{2-2c_1} = \sqrt{c_4+1}$, which leads to $c_4 = 1-2c_1$ and consequently $\sqrt{3c_4} = \sqrt{3-6c_1}$, again making all three ratios identical. Note that by remark 1, we have the bound $-1 < c_1 < 1/2$ corresponding exactly to $0 < c_4 < 3$.

Having verified that the ratios of the edge lengths are the same for the different conditions, we need to show that the tetrahedral configurations formed by the edges are the same. We observe that for each condition the type-II edges contain a pair of edges opposing each other. Any configurations of the type-I and type-III edges for the remaining edges all produce similar tetrahedra, so thus we have that the tetrahedra produced by each of the conditions are equivalent to up to a similarity transform.

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In conclusion, we find that a tetrahedron is subdivision invariant if and only if it satisfies the edge length ratios $1 : x : \sqrt{3x^2 - 3}$, with three edges of length 1, two edges of length x that are opposite to each other, and one edge of length $\sqrt{3x^2 - 3}$, with a bound of $1 < x < 2$ that ensures that the tetrahedron is not degenerate. □

Lemma 3. *A SITet has at least two pairs of opposing congruent dihedral angles. More specifically, it has two dihedral angles equal to 90 degrees along the pair of opposing type-II edges and one dihedral angle equal to 60 degrees along the type-I edge. For the three dihedral angles along type-III edges, the sum of the three angles is 180 degrees, with two congruent angles along a pair of opposing edges, and the remaining angle along the edge opposite to the type-I edge.*

Proof. We first find the normal vector vector $\overrightarrow{v}_i$ of the face opposite point p_i. Using condition 2 for our calculations with $y_2 = c_2$, we get:

$$\overrightarrow{v}_1 = \begin{pmatrix} -2\sqrt{3}c_2 \\ \frac{-2\sqrt{3}}{3} \\ 0 \end{pmatrix}, \ \overrightarrow{v}_2 = \begin{pmatrix} 2\sqrt{3}c_2 \\ -\frac{\sqrt{3}}{3} \\ -1 \end{pmatrix}, \ \overrightarrow{v}_3 = \begin{pmatrix} 0 \\ -\sqrt{3} \\ 1 \end{pmatrix}, \ \overrightarrow{v}_4 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Obviously, $\overrightarrow{v}_1 \cdot \overrightarrow{v}_4 = \overrightarrow{v}_2 \cdot \overrightarrow{v}_3 = 0$. Those vertex pairs correspond to $90°$ dihedral angles along the type-II edges AD and BC. Moreover, $\overrightarrow{v}_3 \cdot \overrightarrow{v}_4 = \|\overrightarrow{v}_3\|\|\overrightarrow{v}_4\|/2$, corresponding to a $60°$ dihedral angle along the type-I edge AB. Let $\phi_{P,Q}$ denote the dihedral angle between the two faces adjacent to edge PQ for any pair of vertices P and Q. We get

$$\cos\phi_{A,C} = \cos\phi_{B,D} = \frac{\sqrt{3}}{\sqrt{36c_2^2 + 4}}, \quad \cos\phi_{C,D} = \frac{18c_2^2 - 1}{18c_2^2 + 2}.$$

Thus,

$$\cos(\phi_{A,C} + \phi_{B,D}) = \cos(2\phi_{A,C}) = 2\cos^2(\phi_{A,C}) - 1 = \frac{-18c_2^2 + 1}{18c_2^2 + 2} = -\cos(\phi_{C,D}).$$

Consequently, we see that $\phi_{A,C} + \phi_{B,D} + \phi_{C,D} = 180°$, with $\phi_{A,C} = \phi_{B,D}$. Moreover, $\phi_{C,D}$, the unique angle in this trio, corresponds to the edge that is opposite to the type-I edge. □

Lemma 4. *A SITet has two sets of two congruent faces, with one of these sets having isosceles faces.*

Proof. We see that, for condition 1, $\Delta\overline{ABD} \cong \Delta\overline{CDB}$ and $\Delta\overline{ABC} \cong \Delta\overline{CAD}$, with side lengths $AB = AC = CD$ giving us two sets of two congruent faces, and one set of them being composed of isosceles triangles. Since the other conditions provide the same structure of equivalent edge lengths, we see that the same results hold. □

4. Optimization studies of subdivision invariant tetrahedra

We seek to find tetrahedra that are "optimal" among all SITet according to various different metrics. It turns out that the second Sommerville tetrahedron (SSTet) introduced earlier plays a special role in much of the discussion.

Let us first document some special properties of SSTet. First of all, we have

Lemma 5. *SSTet are the only SITet with three pairs of equal edges, and the only ones with three pairs of equal dihedral angles. They are also the only ones with two pairs of isosceles faces.*

Proof. Given a SITet, it has necessarily edge ratios $1:1:1:x:x:\sqrt{3x^2-3}$ for $x \in (1,2)$. Having three pairs of equal edges implies that $x = 2/\sqrt{3}$, which corresponds to a SSTet. Similarly, three pairs of equal dihedral angles means, by the proof of the lemma 3 and using condition 2 with the notation $y_2 = c_2$, that

$$\frac{12c_2^2 - \frac{2}{3}}{12c_2^2 + \frac{4}{3}} = \frac{1}{2}\,.$$

This means $36c_2^2 = 8$ and we again get a SSTet. The argument for all faces being isosceles leading to a SSTet is the same as that for three equal edge pairs. □

With regard to mirror symmetry and the use of mirror reflection for congruence, we have the following.

Lemma 6. *SSTet are the only SITet with mirror symmetry (they in fact have two perpendicular planes of symmetry) and they are the only SITet for which the subdivided tetrahedra are properly congruent, that is, congruent with the same orientation order.*

Proof. We consider the condition 2 with $y_2 = c_2$. It is obvious that any plane of mirror symmetry for a tetrahedron must contain two vertices, while the other two vertices must be symmetric with respect to the plane. For configuration given in condition 2, $\overrightarrow{AB}$ cannot be perpendicular to $\overrightarrow{CD}$, so there are only two possibilities: either $\overrightarrow{AC} \perp \overrightarrow{BD}$ or $\overrightarrow{AD} \perp \overrightarrow{BC}$. These orthogonality conditions correspond to equations

$$(\frac{1}{3}, 2c_2, 0)\cdot(-\frac{1}{3}, c_2, \sqrt{3}c_2) = 0 \quad \text{or} \quad (\frac{1}{3}, 2c_2, 0)\cdot(-\frac{1}{3}, c_2, \sqrt{3}c_2) = 0.$$

The only values of c_2 making any of the above satisfied are $c_2^2 = 2/9$, corresponding to SSTet for which both equations are satisfied simultaneously. This proves the first part of the lemma. The second part follows from the discussion given in [37]. □

SSTet also look the most symmetric or regular among SITet in the following sense.

Lemma 7. *SSTet are the only SITet with the circumcenter, inscribed center, and mass centroid being at the same point.*

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Proof. We again use condition 2 as illustration with $y_2 = c_2$. A direct calculation of the mass centroid gives $(1/2, 3c_2/4, \sqrt{3}c_2/4)$, to coincide with the the circumcenter. We need the following properties:

$$(0, 3c_2/4, \sqrt{3}c_2/4) \cdot (1, 0, 0) = 0,$$
$$(1/3, -c_2/4, 2\sqrt{3}c_2/4) \cdot (1/3, 2c_2, 0) = 0,$$
$$(1/6.c_2/4, -\sqrt{3}c_2/4) \cdot (2/3.c_2, \sqrt{3}c_2) = 0\,.$$

These properties are simultaneously satisfied only for $c_2 = \sqrt{2}/3$, which gives us the SSTet. One can check that the mass centroid is also the inscribed center. □

The above results have shown that SSTet are special SITet with additional symmetric geometric features. We now examine many additional optimization properties associated with SSTet.

Lemma 8. *Among SITet, SSTet have the smallest maximum edge ratios.*

Proof. The maximum of edge ratios for a given SITet is given by

$$g(x) = \max\{x, \frac{x}{\sqrt{3x^2-3}}, \sqrt{3x^2-3}\}$$

for $x \in (1, 2)$. A direct calculation shows

$$g(x) = \begin{cases} \frac{x}{\sqrt{3x^2-3}}, & x \in (1, 2/\sqrt{3}), \\ x, & x \in (2/\sqrt{3}, \sqrt{3/2}), \\ \sqrt{3x^2-3}, & x \in (\sqrt{3/2}, 2). \end{cases}$$

Thus, the minimum of $g = g(x)$ is given by $x = 2/\sqrt{3}$, corresponding to a SSTet. □

Studying the optimization among all SITet is worthwhile to pursue as there are many important motivations: although regular simplices often correspond to optima for many criteria, they cannot tile the whole space except in two space dimensions. Thus, forcing tetrahedra to be very close to regular tetrahedra in three dimensions means that there would be a high probability of leaving gaps made of sliver elements [12,24]. With this in mind, we see that while regular triangles may be viewed as optimal two dimensional triangles, regular tetrahedra may not. To search for a universal definition that serves many practical purposes, we may limit candidate optimal tetrahedra by restricting to the class of space-tiling tetrahedra, or more restrictively, SITet. We note that [30] has discussed the optimal orientation-preserving space tiling tetrahedra, and found that the optimal one corresponds to SSTet. Another desirable property for a tetrahedron is being well-centered, a notion discussed in detail in [50] that consists of the set of tetrahedra whose circumcenters are in their interiors. The SSTet are completely well-centered in the sense that not only are they well-centered themselves, but their faces are also well-centered.

Among the most popular quality measures for tetrahedra used in the meshing community is one defined by $Q(e) = R_{in}/h_{max}$ with R_{in} being the radius of the

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inscribed-sphere and h_{max} the longest edge length [6,19,16,36,43,44]. In two dimensions, the maximum of $Q(e)$ is attained for a regular triangle, and generating a mesh with elements that are as close to regular triangles as possible makes sense, as this is as perfect as one can get from many viewpoints. Unfortunately, while regular tetrahedra give maximum values of $Q(e)$ in three dimensions, they are not SITet nor space filling, so we consider optimization of $Q(e)$ within a smaller class of tetrahedra.

Lemma 9. *Among SITet, SSTet have the largest inradius to longest edge ratio.*

Proof. We perform our analysis using condition 2 from Lemma 1 with $y_2 = c_2$. We first calculate that the inradius is given by

$$\frac{3\sqrt{3}c_2}{6 + 2\sqrt{3}\sqrt{1+9c_2^2}}\,.$$

If the longest edge length is given by $AB = 1$, the inradius to longest edge ratio is given by the above function. By direct calculation, we see that the derivative of the above function has a sign equal to the sign of

$$2\sqrt{3} + 18\sqrt{3}c_2^2 + 3\sqrt{1+9c_2^2} - \sqrt{1+9c_2^2}$$

which is clearly non-zero.

If the longest edge length is $BC = AD = \sqrt{36c_2^2+4}/3$, the derivative of the ratio between the inradius to the longest edge has the same sign as

$$2\sqrt{3} + 3\sqrt{1+9c_2^2} - 18c_2^2\sqrt{1+9c_2^2} - \sqrt{1+9c_2^2}\,.$$

Substituting $x = 9c_2^2/2$, we see that the above is zero when $(x-1)(1+2x+4x^2) = 0$, that is, only when $x = 1$, which corresponds to the SSTet, with an inradius to the longest edge ratio given by $\frac{1}{4\sqrt{2}} \approx 0.176777$.

To complete the proof, we compute the inradius to longest length ratio for tetrahedra in limiting cases, i.e. as c_2 goes to 0 and ∞, as well as the boundary case $\frac{\sqrt{36c_2^2+4}}{3} = 1$ where the lengths of AB and of $BC = AD$ become the same. For the two limiting cases, the ratio goes to 0. As for the boundary case, we are led to $c_2 = \frac{\sqrt{5}}{6}$ with the ratio being $\frac{5}{6\sqrt{3}(\sqrt{\frac{5}{3}}+\frac{2\sqrt{5}}{3})} \approx 0.17296$, thus proving that the optimum of the inradius to longest length ratio is achieved by SSTet. □

We may also optimize with respect to the ratio between circumradius and inradius. For SSTet , this gives 3.162278, and for a regular tetrahedron, it gives 3.

Lemma 10. *Among SITet, SSTet have the smallest circumradius/inradius ratio.*

Proof. Using again the condition 2 with $y_2 = c_2$, the circumradius is given by

$$\frac{\sqrt{4 + 99c_2^2 + 1296c_2^4}}{18\sqrt{3}c_2}\,.$$

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Taking the derivative of the circumradius/inradius ratio, we get that it has a sign equal to the sign of

$$11664\sqrt{3}c_2^6 - 8\sqrt{3} - 24\sqrt{1+9c_2^2} - 135\sqrt{3}c_2^2 - 297c_2^2\sqrt{1+9c_2^2}\,.$$

Substituting $x = \sqrt{1+9c_2^2}$, we get the above factors into

$$(x-\sqrt{3})(16\sqrt{3}x^5 + 48x^4 - 33x^2 + 9)\,.$$

As $x > 1$, we see that the second term is always positive, so the derivative of circumradius/inradius is 0 only when $x = \sqrt{3}$, which corresponds to the SSTet with a ratio $\sqrt{10}$. The limiting cases, i.e. as c_2 goes to 0 and ∞, both have ratio going to infinity, so thus the optimum for circumradius/inradius ratio is achieved by SSTet. $\square$

By Lemma 5, we know that SSTet are the only SITet with all isosceles faces. We may also compare the face areas of SITet.

Lemma 11. *Among SITet, SSTet are the only ones with the same face areas.*

Proof. We use the second condition with $y_2 = c_2$. Let us compute the normalized quantity being the cube of the face area standard deviation divided by the square of volume, that gives

$$\frac{\left(4 + 9c_2^2 - 2\sqrt{3}\sqrt{1+9c_2^2}\right)^{3/2}}{8\sqrt{3}c_2}\,.$$

The above is positive unless $c_2 = \frac{\sqrt{2}}{3}$, corresponding to SSTet. $\square$

A scaled surface area to volume ratio criterion can also be devised to assess the regularity of a tetrahedron. To account for size scaling the square root of the surface area and the cubed root of the volume were used in the ratio. This value is minimized with the regular tetrahedron that has a ratio of 2.6843. We now show that the SSTet are the optimal tetrahedra with the smallest scaled surface area to volume ratio among all SITet.

Lemma 12. *Among SITet, SSTet have the smallest scaled surface area to volume ratio.*

Proof. Using condition 2 with $y_2 = c_2$, the surface area is given by

$$\frac{2}{3}c_2(3 + \sqrt{3}\sqrt{1+9c_2^2})$$

and volume is $c_2^2/\sqrt{3}$. The sign of the derivative of the scaled surface area to volume ratio is equal to the sign of

$$648c_2^2 - 24\sqrt{3}\sqrt{1+9c_2^2} - 24 - 216c_2^2$$

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Substituting $x = \sqrt{1+9c_2^2}$, we see that the above is 0 if and only if $(x-\sqrt{3})(2x+\sqrt{3}) = 0$, and as $x > 1$ we see that the derivative is 0 only when $x = \sqrt{3}$, which corresponds to the SSTet with a ratio of $2^{\frac{11}{12}}3^{\frac{1}{3}} \approx 2.723$. The limiting cases, i.e. as c_2 goes to 0 and ∞, both have ratio going to infinity, so thus the optimum for scaled surface area to volume ratio is achieved by SSTet. □

The above result is consistent with the finding in [30].

4.1. *Optimal subdivision invariant tetrahedra*

The above discussions show SSTet uncannily optimize many criteria among SITet. We summarize this in a theorem as the second major finding of this work.

Theorem 2. *Among SITet, SSTet are optimal with respect to a variety of metrics as follows: they have the smallest maximum edge ratios, the smallest scaled surface area to volume ratio, the largest inradius to longest edge ratio, and the largest inradius to circumradius ratio; they are also the only tetrahedra with circumcenter, incenter, and mass centroids coinciding at the same point, the only tetrahedra with all equal face areas, the only tetrahedra with the largest number of equal edge pairs, the largest number of equal dihedral angle pairs, and the largest number of isosceles triangular faces.*

The theorem follows from the lemmas shown before. Obviously, we may consider many more criteria that would demonstrate the SSTet are closest to be regular among all SITet. A regular tetrahedron has zero deviation in edge length, face area, and dihedral angles, and we may consider the deviations of such quantities among all SITet and consider those having the minimum standard deviations as those being closest to regular or optimal. The standard deviations may be normalized to ensure that scaling the size of a tetrahedron has no impact. We have performed both symbolic and numerical computations to verify that standard deviations of edge lengths, dihedral angles, and face angles are minimized among all SITet by SSTet with the corresponding values given approximately by 0.072927 for edge lengths, 14.142136 for dihedral angles, and 7.44497 for face angles. Although the SSTet dihedral angles of $\pi/2$ and $\pi/3$ are very different from the dihedral angle of $cos^{-1}(1/3) \approx 1.23096$ for the regular tetrahedra, and likewise, the face angles of SSTet are $cos^{-1}(1/3) \approx 1.23096$ and $cos^{-1}(1/\sqrt{3}) \approx 0.95532$ and also differ from $\pi/3$ significantly, the fact that SSTet have the minimum standard deviations among SITet further adds to the optimality of SSTet over other SITet.

4.2. *More optimization questions: extreme anisotropy*

The discussions above are mostly concerned with SITet that are as close as possible to be regular or have the lowest aspect ratio. We now look into those SITet with high aspect ratios. Studying these tetrahedra may allow us to utilize SITet in anisotropic

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mesh generation and optimization in cases where needle-like or plate-like tetrahedra are needed to best capture quantities of interest that have different degrees of variability in different directions. Using subdivision invariant tetrahedra ensures that the refined tetrahedra inherit the same strong anisotropy of the original tetrahedra and avoids leaving voids or producing elements that display different anisotropy.

To begin the discussion, we follow [12] to introduce some classifications of tetrahedra based on their edges and faces. For a triangular face with a high aspect ratio, there are only two cases: namely, a dagger if it has one very short edge; and a blade if there is no short edge. For tetrahedra of high aspect ratio, there are more possibilities. First, a tetrahedron that is close to being a line (or needle) can be classified as a spire, spear, spindle, spike, or splinter, depending on how many of its faces are daggers and blades. More specifically, a spire has one small triangle and 4 daggers; a spear and a spike both have two daggers and two blades, but a spear has one long edge, one short edge and 4 medium edges while a spike has 2 long edges, 3 medium ones and 1 short one; a spindle has no short edge so it has 4 blades; and a splinter has two short edges, four long edges, and four daggers. Meanwhile, a tetrahedron that is close to a plane (or plate) can be classified as a wedge, spade, cap, or sliver: a wedge has two vertices close to each other; a spade has one vertex close to another edge; a cap has one vertex close to another face; and a sliver can be projected to form a quadrilateral. The number of long edges with small dihedral angles also increases from 1 to 4 in these four cases.

Specializing to SITet with high aspect ratios, we get the following.

Lemma 13. *SITet can have high aspect ratios, either as spindles with edge ratios close to* $1:1:1:2:2:3$ *and dihedral angles close to* $30^\circ:30^\circ:60^\circ:90^\circ:90^\circ:120^\circ$*, or as wedges formed by two near-regular faces sharing a common edge with the opposing vertices close to each other with dihedral angles close to* $0^\circ:60^\circ:90^\circ:90^\circ:90^\circ:90^\circ$*.*

Proof. We consider condition 2, where we only need to look at the extreme limiting cases corresponding to $c_2 = y_2 \to 0$ and ∞ as all other c_2 have some finite aspect ratio. In the former case, we see that the tetrahedron we get approaches a line segment with the four points evenly spaced, thus giving us a spindle with three edges of length $\frac{1}{3}$, two edges of length $\frac{2}{3}$, and one edge of length 1.

In the latter case, we have a plane-like shape where one edge has a short length, which is precisely a wedge. All of the other edges tend to have the same length and form two near-regular faces. $\square$

It remains an interesting issue, though beyond the scope of this work, to investigate the relations between these anisotropic SITet and the anisotropic CVTs or CVTs in other metrics [21,39] and to determine, for what type of special anisotropic quantities, the special high aspect ratio elements produced by SITet can offer the most effective approximation/representation.

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5. Discussions

SITet and optimal tetrahedra among SITet are not only interesting geometric objects but also useful in broad applications. We focus on implications for optimal tetrahedral meshing as an illustration.

First of all, it is well-known that optimal meshing depends on optimal placement of vertices [2] and optimal connections between vertices to form meshing elements, often via Delaunay triangulation [4,22,49]. There is a strong tie between SSTet and optimal unstructured tetrahedral mesh generation and optimization. In particular, tetrahedral meshes made up by SSTet, as depicted in Figure 2, gives the dual Delaunay triangulation corresponding to optimal centroidal Voronoi tessellations (CVTs) [17,19]. To further clarify, CVTs are Voronoi tessellations [4] whose generators all coincide with the mass centroids of the Voronoi regions. Optimal CVTs are those CVTs with the minimum CVT energy or clustering energy (also called quantization error or mean square error [17,29]). Asymptotically as the number of generators gets larger and larger, Gersho's Conjecture [29] states that the optimal CVT forms a regular tessellation consisting of the replication of a single polytope whose shape depends only on the spatial dimension. For a uniform density, the regular hexagon provides a confirmation of the conjecture in 2D. For 3D, the special CVT (or quantizer) corresponding to the body-centered cubic lattice (its Voronoi regions are the space-filling *truncated octahedra*) is viewed as the optimal CVT [5,18,20]. As stated above, the dual tetrahedra for the dual Delaunay triangulation correspond precisely to SSTet, the subject studied in this work.

Next, note that contrary to the 2D case, the appearance of opposing dihedral angles of $\pi/2$ in the SSTet does not present degeneracy or numerical instability in 3D, especially for the numerical solutions of many typical PDEs. When solving typical elliptic problems, we expect to get the stiffness matrices to be M-matrices on SSTet meshes, thus providing the desirable numerical stability. Numerical simulation of electromagnetic systems based on co-volume or Yee schemes can also be implemented on 3D SSTet type meshes [45]. Moreover, CVDT-like meshes or meshes based on SSTet offer superconvergent properties [11,35] which can be effectively used in many numerical PDE applications.

Finally, to avoid the geometric frustration due to the fact that regular tetrahedra do not fill space, it is natural to explore new alternatives that either utilize a nice tetrahedron that is space-filling or simple space-filling configurations consisting of a patch of nice tetrahedra. With no gaps left to be filled, many of the elements in the interior mesh can be optimized in a harmonious fashion, thus delegating the issue of high quality meshing mostly to optimizing the boundary fitting. The study given in this work addresses the first of these possibilities where the nice tetrahedron is subdivision invariant and is given by the SSTet. When a large portion of a complex geometric domain is filled by patches of SSTet, extra symmetry and structure properties can be utilized even with generically unstructured triangulations [11]. The subdivision invariance offers additional opportunities for developing multilevel

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resolution and fast numerical solvers. Hence, with effective CVT and CVDT construction algorithms already available and nice approximation properties associated with CVDT and SSTet being explored [18], we may argue that for isotropic tetrahedral meshing, SSTet, which make up the optimal CVDT, are strong candidates for optimal tetrahedra and perfect alternatives to regular tetrahedra in three dimension. Such a conclusion distinguishes from some other ones reported in the literature [1] where conventional regular tetrahedra are treated as the optimal choice. Indeed, instead of attempting to produce regular tetrahedra, we advocate, a new paradigm for three dimensional isotropic tetrahedral mesh generation and optimization that is aimed at producing optimal elements given by the SSTet, and can be achieved via the optimization of CVDT.

In closing, with expanding applications of computational geometric modeling and growing interests in data sciences, there is a strong demand for building computational tools and mathematical models that are suitable for high dimensional geometry. Adopting the same geometric concepts developed historically in lower dimensions such as those in two dimensions may not always be effective or appropriate for high dimensional problems. Using the re-examination of basic concepts like regular and optimal tetrahedra as an illustration, we hope that this study helps to motivate further development of new mathematical understandings of higher dimensional geometry and related computational tools.

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