Discrete Comput Geom 36:111–166 (2006)
DOI: 10.1007/s00454-005-1213-z

Discrete & Computational
Geometry

Sphere Packings, IV. Detailed Bounds

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Abstract. This paper is the fourth in a series of six papers devoted to the proof of the Kepler conjecture, which asserts that no packing of congruent balls in three dimensions has density greater than the face-centered cubic packing. In a previous paper in this series, a continuous function f on a compact space was defined, certain points in the domain were conjectured to give the global maxima, and the relation between this conjecture and the Kepler conjecture was established. The function f can be expressed as a sum of terms, indexed by regions on a unit sphere. In this paper detailed estimates of the terms corresponding to general regions are developed. These results form the technical heart of the proof of the Kepler conjecture, by giving detailed bounds on the function f. The results rely on long computer calculations.

Introduction

This paper contains the technical heart of the proof of the Kepler conjecture. Its primary purpose is to obtain good bounds on the score $\sigma_R(D)$ when R is an arbitrary standard region of a decomposition star D. This is particularly challenging, because we have no a priori restrictions on the combinatorial type of the standard region R. It is not known to be bounded by a simple polygon. It is not known to be simply connected. Moreover, there are multitudes of possible geometrical configurations of upright and flat quarters, each scored by a different rule. This paper deals with these complexities and bounds the score $\sigma_R(D)$ in a way that depends on a simple numerical invariant $n(R)$ of R. When R is bounded by a simple polygon, the numerical invariant is simply the number of sides of the polygon. This bound on the score of a standard region represents the turning point of the proof, in the sense that it caps the complexity of a contravening decomposition star, and restrains the combinatorial possibilities. Later in the proof it is instrumental in the complete enumeration of the plane graphs attached to contravening stars.

The first section proves a series of approximations for the score of upright quarters. The strategy is to limit the number of geometrical configurations of upright quarters by showing that a common upper bound (to the scoring function) can be found for quite disparate geometrical configurations of upright quarters. When a general upper bound can be found that is independent of the geometrical details of upright quarters, we say that the upright quarters can be *erased*. (A precise definition of what it means to erase an upright quarter appears below.) There are some upright quarters that cannot be treated in this manner; and this adds some complications to the proofs in this paper.

The second section states the main result of the paper (Theorem 12.1). An initial reduction reduces the proof to the case that the boundary of the given standard region is a polygon. A further argument is presented to reduce the proof to a convex polygon.

The third section completes the proof of the main theorem. This part of the proof relies on a new geometrical decomposition of the part of a V-cell over a standard region. The pieces in this decomposition are called *truncated corner cells*.

A final section in this paper collects miscellaneous further bounds that will be needed in later parts of the proof of the Kepler conjecture.

11. Upright Quarters

11.1. *Erasing Upright Quarters*

Definition 11.1. A standard region is said to be *exceptional* if it is not a triangle or a quadrilateral. The pair (D, R) consisting of a decomposition star and an exceptional standard region is said to be an *exceptional cluster*. The vertices of the packing of height at most $2t_0$ that are contained in the closed cone over the standard region are called its *corners*.

Fix an exceptional cluster R. Throughout this paper, we assume that R lies on a star of score at least $8\,pt$. It is to be understood, when we say that a standard region does not exist, that we mean that there exists no such region on any star scoring more than $8\,pt$.

In this section we discuss how to eliminate many cases of upright diagonals. The results are summarized in Section 11.9.

If R is a standard region, we write $V_R(t)$ for the intersection of the local V-cell $V_R = \mathrm{VC}(0) \cap C(R)$ with a ball $B(t)$, centered at the origin, of radius t. We usually take $t = t_0$. If $\{0, v\}$, of length between $2t_0$ and $2\sqrt{2}$, is not the diagonal of an upright quarter in the Q-system, then v does not affect the truncated cell $V_R(t_0)$ and may be disregarded. For this reason we confine our attention to upright diagonals that lie along an upright quarter in the Q-system.

We say that an upright diagonal $\{0, v\}$ can be *erased with penalty* $\pi_0 \geq 0$, if we have, in terms of the decomposition of Section 9,

$$\sum_Q \sigma(Q) + \sum_S \sigma(V_S(t_S)) - 4\delta_{\mathrm{oct}}\,\mathrm{vol}(\delta_P(v)) < \pi_0 + \sum_Q \text{s-vor}_0(Q) + \sum_S \text{s-vor}_0(S).$$

Here the sum over Q runs over the upright quarters around $\{0, v\}$. The scores $\sigma(Q)$ are context-dependent (see Section 7). The second sum runs over simplices S along $\{0, v\}$ of type C in the $\mathcal{S}$-system. We define their score $\sigma(V_S(t_S))$ as in Section 9. Also, $\delta_P(v)$ is the piece of the decomposition defined in Section 9. The right-hand side is scored by the truncation function in Section 7 (formula (7.13)). When we erase without mention of a penalty, $\pi_0 = 0$ is assumed.

If the diagonal can be erased, an upper bound on the score is obtained by ignoring the upright diagonal and all of the structures around it coming from the decomposition of Section 9, and switching to the truncation at t_0. The current section shows that various vertices can be erased, and this will greatly reduce the number of combinatorial possibilities for an exceptional cluster.

11.2. *Contexts*

Each upright diagonal has a context (p, q), with p the number of anchors and $p - q$ the number of quarters around the diagonal (Definition 7.1). The dihedral angle of a quarter is less than[24] π, so the context (2, 0) is impossible. There is at least one quarter, so $p \geq q + 1$, $p \geq 2$.

The context (2, 1) is treated in Section 10.4. Lemma 10.15 shows that by removing the upright diagonal, and scoring the surrounding region by a truncated function vor_0, an upper bound on the score is obtained. In the remaining contexts, $p \geq 3$. We start with contexts satisfying $p = 3$. The context (3, 0) is to be regarded as two quasi-regular tetrahedra sharing a face rather than as three quarters along a diagonal. In particular, by Definition 4.8, the upright quarters do not belong to the Q-system.

We recall that the score of an upright quarter is given by

$$\sigma(Q, v) = (\mu(Q, v) + \mu(Q, \hat{v}) + \text{s-vor}_0(Q, v) - \text{s-vor}_0(Q, \hat{v}))/2,$$

except in the contexts (2, 1) and (4, 0). Define $\nu(Q)$ to be the right-hand side of this equation. The context (2, 1) has been treated, and the context (4, 0) does not occur in exceptional clusters. Thus, for the remainder of this section, the scoring rule $\sigma(Q) = \nu(Q)$ is used.

We have several different variants on the score depending on the truncation, analytic continuation, and so forth. If f is any of the functions

$$\text{s-vor}_0,\ \text{s-vor},\ \Gamma,\ \nu,$$

we set τ_0, τ_V, τ_Γ, τ_ν, respectively, to

$$\tau_* = -f(S) + \mathrm{sol}(S)\zeta\, pt.$$

We set $\tau(S, t) = -\,\text{s-vor}(S, t) + \mathrm{sol}(S)\zeta\, pt$. The family of functions τ_* measure what is squandered by a simplex. We say that Q has *compression type* or *Voronoi type* according to the scoring of $\mu(Q)$. (See Section 7.1.)

Crowns and anchor correction terms are used in Section 10.4 to erase upright quarters. We imitate those methods here. The functions crown and anc are defined and discussed in Section 10.4. If $S = S(y_1, \ldots, y_6)$ is a simplex along $\{0, v\}$, set

$$\kappa(S(y_1, \ldots, y_6)) = \mathrm{crown}(y_1/2)\,\mathrm{dih}(S)/(2\pi) + \mathrm{anc}(y_1, y_2, y_6) + \mathrm{anc}(y_1, y_3, y_5).$$

[24] CALC-971555266.

$\kappa(S)$ is a bound on the difference in the score resulting from truncation around v. Assume that S is the simplex formed by $\{0, v\}$ and two consecutive anchors around $\{0, v\}$. Assume further that the circumradius of S is at least $\eta_0(y_1/2)$. Then we have

$$\kappa(S) = -4\delta_{\mathrm{oct}}\,\mathrm{vol}(\delta_P(W^e)),$$

where W^e is the extended wedge constructed in Section 9.2. To see this, it is a matter of interpreting the terms in κ. The function *crown* enters the volume through the region over the spherical cap D_0 of Section 9.2, lying outside $B(t_0)$. By multiplying by $\mathrm{dih}(S)/(2\pi)$, we select the part of the spherical cap over the unextended wedge W between the anchors. The terms *anc* adjust for the four Rogers simplices lying above the extension W^e.

11.3. *Three Anchors*

Lemma 11.2. *The upright diagonal can be erased in the context* (3, 2).

Proof. Let v_1 and v_2 be the two anchors of the upright diagonal $\{0, v\}$ along the quarter. Let the third anchor be v_3.

Assume first that $|v| \geq 2.696$. If Q is of compression type, then[25] the score is dominated by the truncated function s-vor$_0$. Assume Q is of Voronoi type. If $|v_1|, |v_2| \leq 2.45$, then a calculation[26] gives the result. Take $|v_2| \geq 2.45$. By symmetry, $|v - v_1|$ or $|v - v_2| \geq 2.45$. The case $|v - v_1| \geq 2.45$ is treated by another calculation.[27] We take $|v - v_2| \geq 2.45$. Let $S = \{0, v, v_2, v_3\}$. If S is of type C, the result follows.[28] S is of type C, if and only if $y_4 \leq 2.77$ (because $\eta_{456} \geq \eta(2.45, 2, 2.77) > \sqrt{2}$). If S is not of type C, we argue as follows. The function $h^2(\eta(2h, 2.45, 2.45)^{-2} - \eta_0(h)^{-2})$ is a quadratic polynomial in h^2 with negative values for $2h \in [2.696, 2\sqrt{2}]$. From this we find

$$\mathrm{rad}(S) \geq \eta(2h, 2.45, 2.45) \geq \eta_0(h), \qquad \text{where} \quad 2h = |v|,$$

and this justifies the use of κ (see Section 9.2, Case (2)). That the truncated function dominates the score now follows from a calculation.[29]

Now assume that $|v| \leq 2.696$. If the simplices $\{0, v, v_1, v_3\}$ and $\{0, v, v_2, v_3\}$ are of type C, the bound follows from a calculation.[30,31] If say $S = \{0, v, v_2, v_3\}$ is not of type C, then

$$\mathrm{rad}(S) \geq \sqrt{2} > \eta_0(2.696/2) \geq \eta_0(h),$$

justifying the use of κ. The bound follows from further calculations.[32–34] ($\Gamma + \kappa <$ octavor$_0$, etc.) □

[25] CALC-73974037.
[26] CALC-764978100.
[27] CALC-764978100.
[28] CALC-764978100.
[29] CALC-618205535.
[30] CALC-73974037.
[31] CALC-764978100.
[32] CALC-618205535.
[33] CALC-73974037.
[34] CALC-764978100.

Lemma 11.3. *The upright diagonal can be erased in the context* (3, 1), *provided the three anchors do not form a flat quarter at the origin.*

Proof. In the absence of a flat quarter, truncate, score, and remove the vertex v as in the context (3, 1) of Lemma 10.15. If there is a flat quarter, by the rules of Definition 4.8, v is enclosed over the flat quarter. We do nothing further with them for now. This unerased case appears in the summary, Section 11.9. See Lemma 11.27. □

11.4. *Six Anchors*

Lemma 11.4. *An upright diagonal has at most five anchors.*

Proof. The proof relies on constants and inequalities from two calculations.[35,36] If between two anchors there is a quarter, then the angle is greater than 0.956, but if there is not, the angle is greater than 1.23. So if there are k quarters and at least six anchors, they squander more than

$$k(1.01104) - [2\pi - (6-k)1.23]0.78701 > (4\pi\zeta - 8)\,pt,$$

for $k \geq 0$. □

11.5. *Anchored Simplices*

Let $\{0, v\}$ be an upright diagonal, and let $v_1, v_2, \ldots, v_k = v_1$ be its anchors, ordered cyclically around $\{0, v\}$. This cyclic order gives dihedral angles between consecutive anchors around the upright diagonal. We define the dihedral angles so that their sum is 2π, even though this will lead us to depart from our usual conventions by assigning a dihedral angle greater than π when all the anchors are concentrated in some half-space bounded by a plane through $\{0, v\}$. When the dihedral angle of $S = \{0, v, v_i, v_{i+1}\}$ is at most π, we say that S is an *anchored simplex* if $|v_i - v_{i+1}| \leq 3.2$. (The constant 3.2 appears throughout this section.) All upright quarters are anchored simplices. If an upright diagonal is completely surrounded by anchored simplices, the upright diagonal is sometimes called a *loop*. If $|v_i - v_{i+1}| > 3.2$ and the angle is less than π, we say there is a *large gap* around $\{0, v\}$ between v_i and v_{i+1}.

To understand how anchored simplices overlap we need a bound satisfied by vertices enclosed over an anchored simplex.

Lemma 11.5. *A vertex w of height between* 2 *and* $2\sqrt{2}$, *enclosed in the cone over an anchored simplex* $\{0, v, v_1, v_2\}$ *with diagonal* $\{0, v\}$ *satisfies* $|w - v| \leq 2t_0$. *In particular, if* $|w| \leq 2t_0$, *then w is an anchor.*

[35] CALC-729988292.
[36] CALC-83777706.

Proof. As in Lemma 4.16, the vertex w cannot lie inside the anchored simplex. If $|v_1 - v_2| \le 2\sqrt{2}$, the result follows from Lemma 5.16. In fact, if $|w| \le 2\sqrt{2}$, the Voronoi cells at 0 and w meet, so that Lemma 5.16 forces $\{0, v_1, v_2, w\}$ to be a quarter. (This observation gives a second proof of Lemma 4.34.)

Assume that a figure exists with $|v_1 - v_2| > 2\sqrt{2}$. Suppose for a contradiction that $|v - w| > 2t_0$. Pivot v_1 around $\{0, v_2\}$ until $|v - v_1| = 2t_0$ and v_2 around $\{0, v_1\}$ until $|v - v_2| = 2t_0$. Rescale w so that $|w| = 2\sqrt{2}$. Set $x = |v_1 - v_2|$. If, through geometric considerations, w is not deformed into the plane of $\{0, v_2, v_1\}$, then we are left with the one-dimensional family $|w'| = |w' - w| = 2$, for $w' = v_2, v_1$, $|v - w| = |v| = |v_1 - v| = |v_2 - v| = 2t_0$, depending on x. This gives a contradiction

$$\begin{aligned}\pi &\ge \mathrm{dih}(v_2, v_1, 0, v) + \mathrm{dih}(v_2, v_1, v, w)\\ &= 2\,\mathrm{dih}(S(x, 2, 2t_0, 2t_0, 2t_0, 2)) > \pi,\end{aligned}$$

for $x > 2\sqrt{2}$. (Equality is attained if $x = 2\sqrt{2}$.)

Thus, we may assume that w lies in the plane $P = \{0, v_1, v_2\}$. Take the circle in P at distance $2t_0$ from v. The vertices 0 and w lie on or outside the circle. The vertices v_1 and v_2 lie on the circle, so the diameter is at least $x > 2\sqrt{2}$. The distance from v to P is less than $x_0 = \sqrt{2t_0^2 - 2}$. The edge $\{0, w\}$ cannot pass through the center of the circle, because $|w|$ is less than the diameter. Reflect v through P to get v'. Then $|v - v'| < 2x_0$. Swapping v_1 and v_2 as necessary, we may assume that w is enclosed over $\{0, v, v', v_2\}$. The desired bound $|v - w| \le 2t_0$ now follows from geometric considerations and the contradiction

$$2\sqrt{2} = |w| > \mathcal{E}(S(2, 2t_0, 2t_0, 2x_0, 2t_0, 2t_0), 2, 2t_0, 2t_0) = 2\sqrt{2}. \qquad \square$$

Corollary 11.6. *A vertex of height at most* $2t_0$ *is never enclosed over an anchored simplex.*

Proof. If so, it would be an anchor to the upright diagonal, contrary to the assumption that the anchored simplex is formed by consecutive anchors. □

11.6. *Anchored Simplices Do Not Overlap*

Definition 11.7. Consider an upright diagonal that is not a loop. Let R be the standard region that contains the upright diagonal and its surrounding quarters. Assume we are in the context $(4, 1)$ or $(5, 1)$. In the context $(4, 1)$, suppose that there does not exist a plane through the upright diagonal such that all three quarters lie in the same half-space bounded by the plane. Then we say that the context is 3-*unconfined*. If such a plane exists, we say that the context is 3-crowded. We call the context $(5, 1)$ a 4-crowded upright diagonal. Sections 11.3 and 11.4 reduce everything to contexts with four or five anchors around each vertex. If there are five anchors, Lemma 11.14 and Remark 11.13 show that we can assume at most one large gap. This gives contexts $(5, 0)$ and $(5, 1)$. If there are four anchors, then Lemma 11.21 will dismiss all contexts except $(4, 0)$ and

(4, 1). Thus, every upright diagonal is exactly one of the following: a loop, 3-unconfined, 3-crowded, or 4-crowded.

Definition 11.8. The Cayley–Menger determinant expresses the volume of a simplex $S(y1, \dots, y_6)$ in the form $\sqrt{\Delta(x_1, \dots, x_6)}/12$, where $x_i = y_i^2$, and Δ is a polynomial with integer coefficients. The polynomial Δ will be used frequently.

This lemma is a consequence of the two others that follow. The context of the lemma is the set of anchored simplices that have not been erased by previous reductions.

Lemma 11.9. *Anchored simplices do not overlap.*

The remaining contexts have four or five anchors. Let w and the anchored simplex $S = \{0, v, v_1, v_2\}$ be as in Section 11.5. Our object is to describe the local geometry when an upright diagonal is enclosed over an anchored simplex. If $|v_1 - v_2| \le 2\sqrt{2}$, we have seen in Lemma 4.32 that there can be no enclosed upright diagonal with four or more anchors over the anchored simplex S.

Assume $|v_1 - v_2| > 2\sqrt{2}$. Let $w_1, \dots, w_k$, $k \ge 4$, be the anchors of $\{0, w\}$, indexed consecutively. The anchors of $\{0, w\}$ do not lie in $C(S)$, and the triangles $\{0, w, w_i\}$ and $\{0, v, v_j\}$ do not overlap. Thus, the plane $\{0, v_1, v_2\}$ separates w from $\{w_1, \dots, w_k\}$. Set $S_i = \{0, w, w_i, w_{i+1}\}$. By a calculation[37]

$$\pi \ge \mathrm{dih}(S_1) + \cdots + \mathrm{dih}(S_{k-1}) \ge (k-1)0.956.$$

Thus, $k = 4$. The common upright diagonal of the three simplices $\{S_i\}$ is 3-*crowded*. We claim that $\{v_1, v_2\} = \{w_1, w_4\}$. Suppose to the contrary that, after reindexing as necessary, $S_0 = \{0, w, w_1, v_1\}$ is a simplex, with $v_1 \ne w_1$, that does not overlap $S_1, \dots, S_3$. Then $\pi \ge \mathrm{dih}(S_0) + \cdots + \mathrm{dih}(S_3)$. So $0.28 \ge \pi - 3(0.956) \ge \mathrm{dih}(S_0)$. A calculation[38] now implies that $|w - v_1| \ge 2\sqrt{2}$.

Assume that $\{0, w, v_1, v_2\}$ are coplanar. Disregard the other vertices. We minimize $|v_1 - v_2|$ when

$$|w| = 2\sqrt{2}, \qquad |v_2| = |v_1| = |w - v_2| = 2, \qquad |w - v_1| = 2\sqrt{2}.$$

This implies $3.2 \ge |v_1 - v_2| \ge x$, where x is the largest positive root of the polynomial $\Delta(8, 4, 4, x^2, 4, 8)$. However, $x \approx 3.36$, a contradiction.

Since $\{0, w, v_1, v_2\}$ cannot be coplanar vertices, geometric considerations apply and

$$2\sqrt{2} \ge |w| \ge \mathcal{E}(S(2, 2, 2, 2, 2, 3.2), 2\sqrt{2}, 2, 2) > 2\sqrt{2}.$$

This contradiction establishes that $v_1 = w_1$.

Lemma 11.10. *Around a* 3-*crowded upright diagonal*, *all of the anchored simplices are quarters*.

[37] CALC-83777706.
[38] CALC-83777706.

Proof. The proof makes use of constants and inequalities from several different calculations.[39–41] The dihedral angles are at most $\pi - 2(0.956) < 1.23$. This forces $y_4 \le 2t_0$, for each simplex S. So they are all quarters. $\square$

Lemma 11.11. *If there is* 3*-crowded upright diagonal*, *then the three anchored simplices squander more than* 0.5606 *and score at most* -0.4339.

Proof. The proof makes use of constants and inequalities from several different calculations.[42–44] The three anchored simplices squander at least

$$3(1.01104) - \pi(0.78701) > 0.5606.$$

The bound on the score follows similarly from $\nu < -0.9871 + 0.80449\,\mathrm{dih}$. $\square$

Lemma 11.12. *If a simplex at a* 3*-crowded upright diagonal overlaps an anchored simplex*, *the decomposition star does not contravene*.

Proof. Suppose that $\{0, v, v_1, v_2\}$ is an anchored simplex that another anchored simplex overlaps, with $\{0, v\}$ the upright diagonal. Let $\{0, w\}$ be a 3-crowded upright diagonal. We score the two simplices $S_i' = \{0, v, w, v_i\}$ by truncation at $\sqrt{2}$. Truncation at $\sqrt{2}$ is justified by face-orientation arguments or by geometric considerations:

$$\mathcal{E}(S(2, 2t_0, 2t_0, 2t_0, 2t_0, 2t_0), 2, 2, 2) > 2\sqrt{2}.$$

A calculation[45] gives

$$\tau_V(S_1', \sqrt{2}) + \tau_V(S_2', \sqrt{2}) \ge 2(0.13) + 0.2(\mathrm{dih}(S_1') + \mathrm{dih}(S_2') - \pi) > 0.26.$$

Together with the three simplices around the 3-crowded upright diagonal that squander at least 0.5606, we obtain the stated bound. $\square$

11.7. *Five Anchors*

When there are five anchors of an upright diagonal, each dihedral angle around the diagonal is at most $2\pi - 4(0.956) < \pi$.

Remark 11.13. There are at most two large gaps by the calculation[46]

$$3(1.65) + 2(0.956) > 2\pi.$$

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[40] CALC-83777706.
[41] CALC-855294746.
[42] CALC-815492935.
[43] CALC-83777706.
[44] CALC-855294746.
[45] CALC-855294746.
[46] CALC-83777706.

Lemma 11.14. *If an upright diagonal has five anchors with two large gaps, then the three anchored simplices squander* $> (4\pi\zeta - 8)\,pt$.

Proof. By a calculation,[47] the anchored simplices are all quarters, $1.23 + 2(1.65) + 2(0.956) > 2\pi$. The dihedral angle is less than $2\pi - 2(1.65)$. The linear programming bound based on various inequalities[48] is greater than $0.859 > (4\pi\zeta - 8)\,pt$. □

Definition 11.15. Define a *masked* flat quarter to be a flat quarter that is not in the Q-system because it overlaps an upright quarter in the Q-system. They can only occur in a very special setting.

Lemma 11.16. *Let* $\{0, v\}$ *be an upright diagonal with at least four anchors. If* Q *is a flat quarter that overlaps an anchored simplex along* $\{0, v\}$, *then the vertices of* Q *are the origin and three consecutive anchors of* $\{0, v\}$.

Proof. For there to be overlap, the diagonal $\{w_1, w_2\}$ of Q must pass through the face $\{0, v, v_1\}$ formed by some anchor v_1 (see Lemma 4.19). By Lemma 4.24, w_1 and w_2 are anchors of $\{0, v\}$. By Lemma 4.32, w_2, v_1, and w_1 are consecutive anchors. If v_1 is a vertex of Q we are done. Otherwise, let $w_3 \neq 0, w_1, w_2$ be the remaining vertex of Q. The edges $\{v, v_1\}$ and $\{v_1, 0\}$ do not pass through the face $\{w_1, w_2, w_3\}$ by Lemma 4.19. Likewise, the edges $\{w_2, w_3\}$ and $\{w_3, w_1\}$ do not pass through the face $\{0, v, v_1\}$. Thus, v is enclosed over the quarter Q.

Let $w_3' \neq w_1, v_1, w_2$ be a fourth anchor of $\{0, v\}$. By Lemma 4.19, we have $w_3' = w_3$. □

Corollary 11.17 (of the proof). *If* v *is enclosed over a flat quarter, then* $\{0, v\}$ *has at most four anchors.*

When we are unable to erase the upright diagonal with five anchors and a large gap, we are able to obtain strong bounds on the score.

Lemma 11.18. *Suppose an upright diagonal in a decomposition star has five anchors and one large gap. The four anchored simplices score at most* -0.25. *The four anchored simplices squander at least* 0.4. *If any of the four anchored simplices is not an upright quarter then the decomposition star does not contravene.*

Proof. A list of inequalities[49] together with[50] $\mathrm{dih} > 1.65$ give the bound -0.25. Further inequalities[51] give the bound 0.4. To get the final statement of the lemma, we again use a series of inequalities.[52,53] □

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[47] CALC-83777706.
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[49] CALC-815492935.
[50] CALC-83777706.
[51] CALC-729988292.
[52] CALC-628964355.
[53] CALC-187932932.

Corollary 11.19. *There is at most one* 4*-crowded upright diagonal in a contravening decomposition star.*

Proof. The crown along the large gap, with the bound of the lemma, gives[54] $0.4 - \kappa \geq 0.4 + 0.02274$ squandered by the upright quarters around a 4-crowded upright diagonal. The rest squanders a positive amount (see Lemma 9.20). If there are two 4-crowded upright diagonals, use $2(0.4 + 0.02274) > (4\pi\zeta - 8)\,pt$. □

Definition 11.20. We set $\xi_\Gamma = 0.01561$, $\xi_V = 0.003521$, $\xi'_\Gamma = 0.00935$, $\xi_\kappa = -0.029$, and $\xi_{\kappa,\Gamma} = \xi_\kappa + \xi_\Gamma = -0.01339$.

The first two constants appear in calculations[55,56] as penalties for erasing upright quarters of compression type, and Voronoi type, respectively. ξ'_Γ is an improved bound on the penalty for erasing when the upright diagonal is at least 2.57. Also, ξ_κ is an upper bound[57] on κ, when the upright diagonal is at most 2.57. If the upright diagonal is at least 2.57, then we still obtain the bound[58] $\xi_{\kappa,\Gamma} = -0.02274 + \xi'_\Gamma$ on the sum of κ with the penalty from erasing an upright quarter.

11.8. *Four Anchors*

Lemma 11.21. *If there are at least two large gaps around an upright diagonal with four anchors, then it can be erased.*

Proof. There are at least as many large gaps as upright quarters. Each large gap drops us by ξ_κ and each quarter lifts us by at most[59–61] ξ_Γ. We have $\xi_{\kappa,\Gamma} < 0$. □

Remark 11.22. Let $\{0, v\}$ be an enclosed vertex over a flat quarter. Then

$$|v| \geq \mathcal{E}(2, 2, 2, 2t_0, 2t_0, 2\sqrt{2}, 2, 2, 2) > 2.6.$$

If an edge of the flat quarter is sufficiently short, say $y_6 \leq 2.2$, then

$$|v| \geq \mathcal{E}(2, 2, 2, 2.2, 2t_0, 2\sqrt{2}, 2, 2, 2) > 2.7.$$

The two dihedral angles on the gaps are > 1.65. If the two quarters mask a flat quarter, we use the scoring of 2(c) in Section 11.9. We have $0.0114 < -2\xi_{\kappa,\Gamma}$.

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[55] CALC-73974037.
[56] CALC-764978100.
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[58] CALC-618205535.
[59] CALC-618205535.
[60] CALC-73974037.
[61] CALC-764978100.

When there is one large gap, we may erase with a penalty $\pi_0 = 0.008$.

Lemma 11.23. *Let v be an upright diagonal with four anchors. Assume that there is one large gap. The anchored simplices can be erased with penalty* $\pi_0 = 0.008$. *If any of the anchored simplices around v is not an upright quarter then we can erase with penalty* $\pi_0 = 0.00222$.

Moreover, if there is a flat quarter overlapping an upright quarter, then one of the following holds:

(1) *The truncated function* s-vor$_0$ *exceeds the score by at least* 0.0063. *The diagonal of the flat is at least* 2.6, *and the edge opposite the diagonal is at least* 2.2.
(2) *The truncated function exceeds the score by at least* 0.0114. *The diagonal of the flat is at least* 2.7, *and the edge opposite the diagonal is at most* 2.2.

Definition 11.24. Let a 3-unconfined upright diagonal be an upright diagonal that has four anchors and one large gap in a situation where there is no masked flat quarter.

Proof. The constants and inequalities used in this proof can be found in a series of calculations.[62–64]

First we establish the penalty 0.008. The truncated function s-vor$_0$ is an upper bound on the score of an anchored simplex that is not a quarter. By these inequalities, the result follows if the diagonal satisfies $y_1 \geq 2.57$.

Take $y_1 \leq 2.57$. If any of the upright quarters are of Voronoi type, the result follows from $(\xi_{\kappa,\Gamma} + \xi_\Gamma < 0.008)$. If the edges along the large gap are less than 2.25, the result follows from $(-0.03883 + 3\xi_\Gamma = 0.008)$. If all but one edge along the large gap are less than 2.25, the result follows from $(-0.0325 + 2\xi_\Gamma + 0.00928 = 0.008)$.

If there are at least two edges along the large gap of length at least 2.25, we consider two cases according to whether they lie on a common face of an upright quarter. The same group of inequalities gives the result. The bound 0.008 is now fully established.

Next we prove that we can erase with penalty 0.00222, when one of the anchored simplices is not a quarter. If $|v| \geq 2.57$, then we use

$$2\xi_\Gamma + \xi_V + \xi_\kappa \leq 0.00935 + 0.003521 - 0.2274 \leq 0.$$

If $|v| \leq 2.57$, we use

$$2(0.01561) - 0.029 \leq 0.00222.$$

Let $v_1 \ldots, v_4$ be the consecutive anchors of the upright diagonal $\{0, v\}$ with $\{v_1, v_4\}$ the large gap. Suppose $|v_1 - v_3| \leq 2\sqrt{2}$.

[62] CALC-618205535.
[63] CALC-73974037.
[64] CALC-764978100.

We claim the upright diagonal $\{0, v\}$ is not enclosed over $\{0, v_1, v_2, v_3\}$. Assume the contrary. The edge $\{v_1, v_3\}$ passes through the face $\{0, v, v_4\}$. Disregarding the vertex v_2, by geometric considerations, we arrive at the rigid figure

$$|v| = 2\sqrt{2}, \qquad |v_1| = |v_1 - v| = |v - v_3| = |v_3| = |v_3 - v_4| = 2,$$
$$|v - v_4| = |v_4| = 2t_0, \qquad |v_1 - v_4| = 3.2.$$

The dihedral angles of $\{0, v, v_1, v_4\}$ and $\{0, v, v_3, v_4\}$ are

$$\mathrm{dih}(S(2\sqrt{2}, 2, 2t_0, 3.2, 2t_0, 2)) > 2.3, \qquad \mathrm{dih}(S(2\sqrt{2}, 2, 2t_0, 2, 2t_0, 2)) > 1.16.$$

The sum is greater than π, contrary to the claim that the edge $\{v_1, v_3\}$ passes through the face $\{0, v, v_4\}$. (This particular conclusion leads to the corollary cited at the end of the proof.) Thus, $\{v_1, v_3\}$ passes through $\{0, v, v_2\}$ so that the simplices $\{0, v, v_1, v_2\}$ and $\{0, v, v_2, v_3\}$ are of Voronoi type.

To complete the proof of the lemma, we show that when there is a masked flat quarter, either (1) or (2) holds. Suppose we mask a flat quarter $Q' = \{0, v_1, v_2, v_3\}$. We have established that $\{v_1, v_3\}$ passes through the face $\{0, v, v_2\}$. To establish (1) assume that $|v_2| \geq 2.2$. The remark before the lemma gives

$$|v_1 - v_3| \geq \mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2t_0, 2t_0), 2, 2, 2) > 2.6.$$

The bound 0.0063 comes from

$$\xi_{\kappa,\Gamma} + 2\xi_V < -0.0063$$

To establish (2) assume that $|v_2| \leq 2.2$. The remark gives

$$|v_1 - v_3| \geq \mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2.2, 2t_0), 2, 2, 2) > 2.7.$$

If the simplex $\{0, v, v_3, v_4\}$ is of Voronoi type, then

$$\xi_\kappa + 3\xi_V < -0.0114.$$

Assume that $\{0, v, v_3, v_4\}$ is of compression type. We have

$$-0.004131 + \xi_{\kappa,\Gamma} + \xi_V \leq -0.0114. \qquad \square$$

Corollary 11.25 (of the proof). *If there are four anchors and if the upright diagonal is enclosed over a flat quarter, then there are four anchored simplices and at least three quarters around the upright diagonal.*

11.9. *Summary*

The following index summarizes the cases of upright quarters that have been treated in this section. If the number of anchors is the number of anchored simplices (no large gaps), the results appear in Section 13.12. Every other possibility has been treated.

- None, one, or two anchors. (Section 11.2.)
- Three anchors: (Section 11.3.)
  - context (3, 0),
  - context (3, 1),
  - context (3, 2),
  - context (3, 3).
- Four anchors. (Section 11.8.)
  - No gaps (Section 13.12),
  - One gap,
  - Two or more gaps.
- Five anchors: (Section 11.7),
  - No gaps (Section 13.12),
  - One gap (4-crowded),
  - Two or more gaps.
- Six or more anchors. (Section 11.4.)

By truncation and various comparison lemmas, we have entirely eliminated upright diagonals except when there are between three and five anchors. We may assume that there is at most one large gap around the upright diagonal.

1. Consider an anchored simplex Q around a remaining upright diagonal. The score is $\nu(Q)$ if Q is a quarter, the analytic function s-vor(Q) if the simplex is of type C (Section 9.4), and the truncated function s-vor$_0(Q)$ otherwise.
2. Consider a flat quarter Q in an exceptional cluster. An upper bound on the score is obtained by taking the maximum of all of the following functions that satisfy the stated conditions on Q. Let y_4 denote the length of the diagonal and y_1 be the length of the opposite edge.
   (a) The function $\mu(Q)$.
   (b) s-vor$_0(Q) - 0.0063$, if $y_4 \geq 2.6$ and $y_1 \geq 2.2$. (Lemma 11.23.)
   (c) s-vor$_0(Q) - 0.0114$, if $y_4 \geq 2.7$ and $y_1 \leq 2.2$. (Lemma 11.23.)
   (d) $\nu(Q_1) + \nu(Q_2) +$ s-vor$_x(S)$, if there is an enclosed vertex v over Q of height between $2t_0$ and $2\sqrt{2}$ that partitions the convex hull of (Q, v) into two upright quarters Q_1, Q_2 and a third simplex S. Here s-vor$_x =$ s-vor if S is of type C, and s-vor$_x =$ s-vor$_0$ otherwise. (Lemma 11.3.)
   (e) s-vor$(Q, 1.385)$ if the simplex is of type B (Section 9.4.)
   (f) s-vor$_0(Q)$ if the simplex is an isolated quarter with $\max(y_2, y_3) \geq 2.23$, $y_4 \geq 2.77$, and $\eta_{456} \geq \sqrt{2}$.
3. If S is a simplex is of type A, its score is s-vor(S). (Section 9.4.)
4. Everything else is scored by the truncation vor$_0$. Formula (7.13) is used on these remaining pieces. On top of what is obtained for the standard cluster by summing all these terms, there is a penalty $\pi_0 = 0.008$ each time a 3-unconfined upright diagonal is erased.
5. The remaining upright diagonals that are not completely surrounded by anchored simplices are 3-unconfined, 3-crowded, or 4-crowded from Sections 11.6–11.8.

11.10. *Some Flat Quarters*

Recall that $\xi_V = 0.003521$, $\xi_\Gamma = 0.01561$, and $\xi'_\Gamma = 0.00935$. They are the penalties that result from erasing an upright quarter of Voronoi type, an upright quarter of compression type, and an upright quarter of compression type with diagonal ≥ 2.57. (See calculations.[65,66])

In the next lemma we score a flat quarter by any of the functions on the given domains

$$\hat\sigma = \begin{cases} \Gamma, & \eta_{234}, \eta_{456} \le \sqrt{2}, \\ \text{s-vor}, & \eta_{234} \ge \sqrt{2}, \\ \text{s-vor}_0, & y_4 \ge 2.6,\ \ y_1 \ge 2.2, \\ \text{s-vor}_0, & y_4 \ge 2.7, \\ \text{s-vor}_0, & \eta_{456} \ge \sqrt{2}. \end{cases}$$

Lemma 11.26. *$\hat\sigma$ is an upper bound on the functions in* 2(a)–(f) *of Section* 11.9. *That is, each function is dominated by some choice of $\hat\sigma$.*

Proof. The only case in doubt is the function of 3.10(d):

$$\nu(Q_1) + \nu(Q_2) + \text{s-vor}_x(S).$$

This is established by the following lemma. ☐

We consider the context (3, 1) that occurs when two upright quarters in the Q-system lie over a flat quarter. Let $\{0, v\}$ be the upright diagonal, and assume that $\{0, v_1, v_2, v_3\}$ is the flat quarter, with diagonal $\{v_2, v_3\}$. Let σ denote the score of the upright quarters and other anchored simplex lying over the flat quarter.

Lemma 11.27. $\sigma \le \min(0, \text{s-vor}_0)$.

Proof. The bound of 0 is established in Theorem 8.4.

By a calculation,[67] if $|v| \ge 2.69$, then the upright quarters satisfy

$$\nu < \text{s-vor}_0 + 0.01(\pi/2 - \text{dih}),$$

so the upright quarters can be erased. Thus we assume without loss of generality that $|v| \le 2.69$.

We have

$$|v| \ge \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 2\sqrt{2}), 2, 2, 2) > 2.6.$$

If $|v_1 - v_2| \le 2.1$, or $|v_1 - v_3| \le 2.1$, then

$$|v| \ge \mathcal{E}(S(2, 2, 2, 2.1, 2t_0, 2\sqrt{2}), 2, 2, 2) > 2.72,$$

[65] CALC-73974037.
[66] CALC-764978100.
[67] CALC-855677395.

contrary to assumption. So take $|v_1 - v_2| \geq 2.1$ and $|v_1 - v_3| \geq 2.1$. Under these conditions we have the interval calculation[68] $\nu(Q) <$ s-vor$_0(Q)$ where Q is the upright quarter. $\square$

Remark 11.28. If we have an upright diagonal enclosed over a masked flat quarter in the context (4, 1), then there are three upright quarters. By the same argument as in the lemma, the two quarters over the masked flat quarter score $\leq$ s-vor$_0$. The third quarter can be erased with penalty ξ_V.

Define the *central vertex* v of a flat quarter to be the vertex for which $\{0, v\}$ is the edge opposite the diagonal.

Lemma 11.29. $\mu <$ s-vor$_0 + 0.0268$ *for all flat quarters. If the central vertex has height* ≤ 2.17, *then* $\mu <$ s-vor$_0 + 0.02$.

Proof. This is an interval calculation.[69] $\square$

We measure what is squandered by a flat quarter by $\hat{\tau} = \mathrm{sol}\,\zeta pt - \hat{\sigma}$.

Lemma 11.30. *Let v be a corner of an exceptional cluster at which the dihedral angle is at most* 1.32. *Then the vertex v is the central vertex of a flat quarter Q in the exceptional region. Moreover,* $\hat{\tau}(Q) > 3.07\,pt$. *If* $\hat{\sigma} =$ s-vor$_0$ (*and if* $\eta_{456} \geq \sqrt{2}$), *we may use the stronger constant* $\tau_0(Q) > 3.07\,pt + \xi_V + 2\xi'_\Gamma$.

Proof. Let $S = S(y_1, \ldots, y_6)$ be the simplex inside the exceptional cluster centered at v, with $y_1 = |v|$. The inequality dih ≤ 1.32 gives the interval calculation $y_4 \leq 2\sqrt{2}$, so S is a quarter. The result now follows by interval arithmetic.[70] $\square$

12. Bounds in Exceptional Regions

12.1. *The Main Theorem*

Let (R, D) be a standard cluster. Let U be the set of corners, that is, the set of vertices in the cone over R that have height at most $2t_0$. Consider the set E of edges of length at most $2t_0$ between vertices of U. We attach a multiplicity to each edge. We let the multiplicity be 2 when the edge projects radially to the interior of the standard region, and 0 when the edge projects radially to the complement of the standard region. The other edges, those bounding the standard region, are counted with multiplicity 1.

Let n_1 be the number of edges in E, counted with multiplicities. Let c be the number of classes of vertices under the equivalence relation $v \sim v'$ if there is a sequence of edges

[68] CALC-148776243.
[69] CALC-148776243.
[70] CALC-148776243.

in E from v to v'. Let $n(R) = n_1 + 2(c-1)$. If the standard region under R is a polygon, then $n(R)$ is the number of sides.

Theorem 12.1. *Let D be a contravening decomposition star. $\tau_R(D) > t_n$, where $n = n(R)$ and*

$$t_4 = 0.1317, \qquad t_5 = 0.27113, \qquad t_6 = 0.41056,$$
$$t_7 = 0.54999, \qquad t_8 = 0.6045.$$

The decomposition star scores less than $8\,pt$, if $n(R) \geq 9$, for some standard cluster R. The scores satisfy $\sigma_R(D) < s_n$, for $5 \leq n \leq 8$, where

$$s_5 = -0.05704, \qquad s_6 = -0.11408, \qquad s_7 = -0.17112, \qquad s_8 = -0.22816.$$

Sometimes, it is convenient to calculate these bounds as a multiple of pt. We have

$$t_4 > 2.378\,pt, \qquad t_5 > 4.896\,pt, \qquad t_6 > 7.414\,pt,$$
$$t_7 > 9.932\,pt, \qquad t_8 > 10.916\,pt.$$

$$s_5 < -1.03\,pt, \qquad s_6 < -2.06\,pt, \qquad s_7 < -3.09\,pt, \qquad s_8 < -4.12\,pt.$$

Corollary 12.2. *Every standard region is a either a polygon or one shown in Fig.* 12.1.

In the cases that are not (simple) polygons, we call the *polygonal hull* the polygon obtained by removing the internal edges and vertices. We have $m(R) \leq n(R)$, where the constant $m(R)$ is the number of sides of the polygonal hull.

Proof. By the theorem, if the standard region is not a polygon, then $8 \geq n_1 \geq m \geq 5$. (Quad clusters and quasi-regular tetrahedra have no enclosed vertices. See Lemmas 10.4 and 5.13.) If $c > 1$, then $8 \geq n = n_1 + 2(c-1) \geq 5 + 2(c-1)$, so $c = 2$, and $n_1 = 5, 6$ (frames 2 and 5 of the figure).

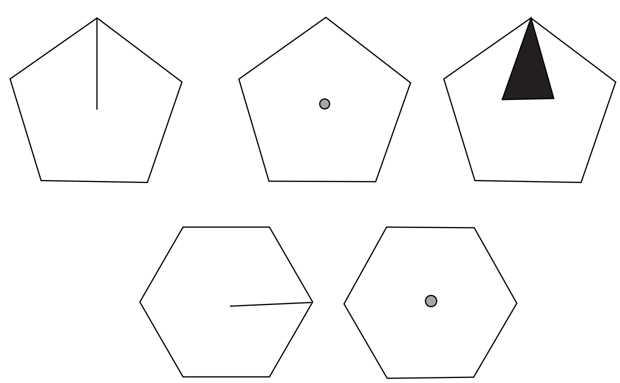

Fig. 12.1

Now take $c = 1$. Then $8 \geq n \geq 5 + (n - m)$, so $n - m \leq 3$. If $n - m = 3$, we get frame 3. If $n - m = 2$, we have $8 \geq m + 2 \geq 5 + 2$, so $m = 5, 6$ (frames 1 and 4).

However, $n - m = 1$ cannot occur, because a single edge that does not bound the polygonal hull has even multiplicity. Finally, if $n - m = 0$, we have a polygon. □

Corollary 12.3. *If the type of a vertex of a decomposition star is* $(7, 0)$, *then it does not contravene.*

Proof. By Theorem 12.1, if there is a nontriangular region, we have

$$\tau(D) \geq \tau_{\mathrm{LP}}(7, 0) + t_4 > (4\pi\zeta - 8)\,pt.$$

Assume that all standard regions are triangular. If there is a vertex that does not lie on one of seven triangles, we have, by Lemma 10.5,

$$\tau(D) \geq \tau_{\mathrm{LP}}(7, 0) + 0.55\,pt > (4\pi\zeta - 8)\,pt.$$

Thus, all vertices lie on one of the seven triangles. The complement of these seven triangles is a region triangulation by five standard regions. There is some vertex of these five that does not lie on any of the other four standard regions in the complement. That vertex has type (3, 0), which is contrary to Lemma 10.9. □

12.2. *Nonagons*

A few additional comments are needed to eliminate $n = 9$ and 10, even after the bounds t_9, t_{10} are established.

Lemma 12.4. *Let F be a set of one or more standard regions bounded by a simple polygon with at most nine edges. Assume that*

$$\sigma_F(D) \leq s_9 \quad \textit{and} \quad \tau_F(D) \geq t_9,$$

where $s_9 = -0.1972$ *and* $t_9 = 0.6978$. *Then D does not contravene.*

Proof. Suppose that $n = 9$, and that R squanders at least t_9 and scores less than s_9. This bound is already sufficient to conclude that there are no other standard clusters except quasi-regular tetrahedra ($t_9 + t_4 > (4\pi\zeta - 8)\,pt$). There are no vertices of type (4, 0) or (6, 0): $t_9 + 4.14\,pt > (4\pi\zeta - 8)\,pt$ by Lemma 10.5. So all vertices not over the exceptional cluster are of type (5, 0). Suppose that there are ℓ vertices of type (5, 0). The polygonal hull of R has $m \leq 9$ edges. There are $m - 2 + 2\ell$ quasi-regular tetrahedra. If $\ell \leq 3$, then, by Lemma 10.6, the score is less than

$$s_9 + (m - 2 + 2\ell)\,pt - 0.48\ell\,pt < 8\,pt.$$

If, on the other hand, $\ell \geq 4$, the decomposition star squanders more than

$$t_9 + 4(0.55)\,pt > (4\pi\zeta - 8)\,pt. \qquad □$$

The bound s_9 will be established as part of the proof of Theorem 12.1.

The case $n = 10$ is similar. If $\ell = 0$, the score is less than $(m-2)\,pt \le 8\,pt$, because the score of an exceptional cluster is strictly negative, Theorem 8.4. If $\ell > 0$, we squander at least $t_{10} + 0.55\,pt > (4\pi\zeta - 8)\,pt$ (Lemma 10.6).

12.3. *Distinguished Edge Conditions*

Take an exceptional cluster. We prepare the cluster by erasing upright diagonals, including those that are 3-unconfined, 3-crowded, or 4-crowded. The only upright diagonals that we leave unerased are loops. When the upright diagonal is erased, we score with the truncated function vor_0 away from flat quarters. Flat quarters are scored with the function $\hat{\sigma}$. The exceptional clusters in Sections 12 and 13 are assumed to be prepared in this way.

A simplex S is *special* if the fourth edge has length at least $2\sqrt{2}$ and at most 3.2, and the others have length at most $2t_0$. The fourth edge is called its diagonal.

We draw a system of edges between vertices. Each vertex will have height at most $2t_0$. The radial projections of the edges to the unit sphere will divide the standard region into subregions. We call an edge *nonexternal* if the radial projection of the edge lies entirely in the (closed) exceptional region.

1. Draw all nonexternal edges of length at most $2\sqrt{2}$ except those between non-consecutive anchors of a remaining upright diagonal. These edges do not cross (Lemma 4.30). These edges do not cross the edges of anchored simplices (Lemmas 4.22 and 4.24).
2. Draw all edges of (remaining) anchored upright simplices that are opposite the upright diagonal, except when the edge gives a special simplex. The anchored simplices do not overlap (Lemma 11.9), so these edges do not cross. These edges are nonexternal (Lemmas 11.5 and 4.19).
3. Draw as many additional nonexternal edges as possible of length at most 3.2 subject to not crossing another edge, not crossing any edge of an anchored simplex, and not being the diagonal of a special simplex.

We fix once and for all a maximal collection of edges subject to these constraints. Edges in this collection are called *distinguished* edges. The radial projection of the distinguished edges to the unit sphere gives the bounding edges of regions called the *subregions*. Each standard region is a union of subregions. The vertices of height at most $2t_0$ and the vertices of the remaining upright diagonals are said to form a *subcluster*.

By construction, the special simplices and anchored simplices around an upright quarter form a subcluster. Flat quarters in the Q-system, flat quarters of an isolated pair, and simplices of type A and B are subclusters. Other subclusters are scored by the function vor_0. For these subclusters, formula (7.13) extends without modification.

12.4. *Scoring Subclusters*

The terms of formula (7.13) defining $\mathrm{vor}_{0,P}(D) = \mathrm{vor}_P(D, t_0)$ have a clear geometric interpretation as quoins, wedges of t_0-cones, and solid angles (see Section 7). There is a quoin for each Rogers simplex. There is a somewhat delicate point that arises in connection with the geometry of subclusters. It is not true in general that the Rogers simplices entering into the truncation $\mathrm{vor}_{0,P}(D)$ of (P, D) lie in the cone over P. Formula (7.13) should be viewed as an analytic continuation that has a nice geometric interpretation when things are nice, and which always gives the right answer when summed over all the subclusters in the cluster, but which may exhibit unusual behavior in general. The following lemma shows that the simple geometric interpretation of formula (7.13) is valid when the subregion is not triangular.

Lemma 12.5. *If a subregion is not a triangle and is not the subregion containing the anchored simplices around an upright diagonal, the cone of arcradius*

$$\psi = \arccos(|v|/(2t_0))$$

centered along $\{0, v\}$, *where* v *is a corner of the subcluster, does not cross out of the subregion.*

Proof. For a contradiction, let $\{v_1, v_2\}$ be a distinguished edge that the cone crosses. If both edges $\{v, v_1\}$ and $\{v, v_2\}$ have length less than $2t_0$, there can be no enclosed vertex w of height at most $2t_0$, unless its distance from v_1 and v_2 is less than $2t_0$:

$$\mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 3.2), 2t_0, 2, 2) > 2t_0.$$

In this case we can replace $\{v_1, v_2\}$ by an edge of the subregion closer to v, so without loss of generality we may assume that there are no enclosed vertices when both edges $\{v, v_1\}$ and $\{v, v_2\}$ have length less than $2t_0$.

The subregion is not a triangle, so $|v-v_1| \geq 2t_0$, or $|v-v_2| \geq 2t_0$, say $|v-v_1| \geq 2t_0$. Also $|v - v_2| \geq 2$. Pivot so that $|v_1 - v_2| = 3.2$, $|v - v_1| = 2t_0$, and $|v - v_2| = 2$. (The simplex $\{0, v_1, v_2, v\}$ cannot collapse ($\Delta \neq 0$) as we pivot. For more details about why $\Delta \neq 0$, see inequality (12.2) in Section 12.7.) Then use[71] $\beta_\psi \leq \mathrm{dih}_3$. □

As a consequence, in nonspecial standard regions, the terms in the formula (7.13) for vor_0 retain their interpretations as quoins, Rogers simplices, t_0-cones, and solid angles, all lying in the cone over the standard region.

12.5. *Proof*

The proof of the theorem occupies the rest of the section. The inequalities for triangular and quadrilateral regions have already been proved. The bounds on t_3, t_4, s_3, and s_4 are found in Lemma 10.1, Section 11.1, Lemma 8.10, and Theorem 8.4, respectively. Thus, we may assume throughout the proof that the standard region is exceptional

We begin with a slightly simplified account of the method of the proof. Set $t_9 = 0.6978$, $t_{10} = 0.7891$, $t_n = (4\pi\zeta - 8)\,pt$, for $n \geq 11$. Set $D(n, k) = t_{n+k} - 0.06585\,k$, for $0 \leq k \leq n$, and $n + k \geq 4$. This function satisfies

$$D(n_1, k_1) + D(n_2, k_2) \geq D(n_1 + n_2 - 2, k_1 + k_2 - 2). \tag{12.1}$$

[71] CALC-193836552.

In fact, this inequality unwinds to $t_r + 0.13943 \geq t_{r+1}$, $D(3,2) = 0.13943$, and $t_n = (0.06585)2 + (n-4)D(3,2)$, for $n = 4, 5, 6, 7$. These hold by inspection.

Call an edge between two vertices of height at most $2t_0$ *long* if it has length greater than $2t_0$. Add the distinguished edges to break the standard regions into subregions. We say that a subregion has *edge parameters* (n, k) if there are n bounding edges, where k of them are long. (We count edges with multiplicities as in Section 12.1, if the subregion is not a polygon.) Combining two subregions of edge parameters (n_1, k_1) and (n_2, k_2) along a long edge e gives a union with edge parameters $(n_1 + n_2 - 2, k_1 + k_2 - 2)$, where we agree not to count the internal edge e that no longer bounds. Inequality (12.1) localizes the main theorem to what is squandered by subclusters. Suppose we break the standard cluster into groups of subregions such that if the group has edge parameters (n, k), it squanders at least $D(n, k)$. Then by superadditivity (formula (12.1)), the full standard cluster R must squander $D(n, 0) = t_n$, $n = n(R)$, giving the result.

Similarly, define constants $s_4 = 0$, $s_9 = -0.1972$, $s_n = 0$, for $n \geq 10$. Set $Z(n, k) = s_{n+k} - k\varepsilon$, for $(n, k) \neq (3, 1)$, and $Z(3, 1) = \varepsilon$, where[72] $\varepsilon = 0.00005$. The function $Z(n, k)$ is subadditive:

$$Z(n_1, k_1) + Z(n_2, k_2) \leq Z(n_1 + n_2 - 2, k_1 + k_2 - 2).$$

In fact, this easily follows from $s_a + s_b \leq s_{a+b-4}$, for $a, b \geq 4$, and $\varepsilon > 0$. It will be enough in the proof of Theorem 12.1 to show that the score of a union of subregions with edge parameters (n, k) is at most $Z(n, k)$.

12.6. *Preparation of the Standard Cluster*

Fix a standard cluster. We return to the construction of subregions and distinguished edges, to describe the penalties. Take the penalty of 0.008 for each 3-unconfined upright diagonal. Take the penalty $0.03344 = 3\xi_\Gamma + \xi_{\kappa,\Gamma}$ for 4-crowded upright diagonals. Take the penalty $0.04683 = 3\xi_\Gamma$ for 3-crowded upright diagonals. Set $\pi_{\max} = 0.06688$. The penalty in the next lemma refers to the combined penalty from erasing all 3-unconfined, 3-crowded, and 4-crowded upright diagonals in the decomposition star. The upright quarters that completely surround an upright diagonal (loops) are not erased.

Lemma 12.6. *The total penalty from a contravening decomposition star is at most* $\pi_{\max}$.

Proof. Before any upright quarters are erased, each quarter squanders[73] > 0.033, so the star squanders $> (4\pi\zeta - 8)\,pt$ if there are twenty-five or more quarters. Assume there are at most twenty-four quarters. If the only penalties are 0.008, we have $8(0.008) < \pi_{\max}$. If we have the penalty 0.04683, there are at most seven other quarters $(0.5606 + 8(0.033) > (4\pi\zeta - 8)\,pt)$ (Lemma 11.11), and no other penalties from this type or from 4-crowded upright diagonals, so the total penalty is at most $2(0.008) + 0.04683 < \pi_{\max}$.

[72] Compare CALC-193836552.
[73] CALC-148776243.

Finally, if there is one 4-crowded upright diagonal, there are at most twelve other quarters (Section 11.7), and erasing gives the penalty $0.03344 + 4(0.008) < \pi_{\max}$. □

The remaining upright diagonals are surrounded by anchored simplices. If the edge opposite the diagonal in an anchored simplex has length $\geq 2\sqrt{2}$, then there may be an adjacent special simplex whose diagonal is that edge. Section 13.12 will give bounds on the aggregate of these anchored simplices and special simplices. In all other contexts, the upright quarters have been erased with penalties.

Break the standard cluster into subclusters as in Section 12.3. If the subregion is a triangle, we refer to the bounds of Section 13.8. Sections 12.7–13.11 give bounds for subregions that are not triangles in which all the upright quarters have been erased. We follow the strategy outlined in Section 12.5, although the penalties will add certain complications.

We now assume that we have a subcluster without quarters and whose region is not triangular. The truncated function vor_0 is an upper bound on the score. Penalties are largely disregarded until Section 13.4.

We describe a series of deformations of the subcluster that increase $\mathrm{vor}_{0,P}(D)$ and decrease $\tau_{0,P}(D)$. These deformations disregard the broader geometric context of the subcluster. Consequently, we cannot claim that the deformed subcluster exists in any decomposition star D. As the deformation progresses, an edge $\{v_1, v_2\}$, not previously distinguished, can emerge with the properties of a distinguished edge. If so, we add it to the collection of distinguished edges, use it if possible to divide the subcluster into smaller subclusters, and continue to deform the smaller pieces. When triangular regions are obtained, they are set aside until Section 13.8.

12.7. *Reduction to Polygons*

By deformation we can produce subregions whose boundary is a polygon. Let U be the set of vertices over the subregion of height $\leq 2t_0$. As in Section 12.1, the distinguished edges partition U into equivalence classes. Move the vertices in one equivalence class U_1 as a rigid body preserving heights until the class comes sufficiently close to form a distinguished edge with another subset. Continue until all the vertices are interconnected by paths of distinguished edges. vor_0 and τ_0 are unchanged by these deformations.

If some vertex v is connected to three or more vertices by distinguished edges, it follows from the connectedness of the open subregion that there is more than one connected component U_i (by paths of distinguished edges) of $U\setminus\{v\}$. Move $U_1 \cup \{v\}$ rigidly preserving heights and keeping v fixed until a distinguished edge forms with another component. Continue until the distinguished edges break the subregions into subregions with polygon boundaries. Again vor_0 and τ_0 are unchanged.

By the end of Section 12, we will deform all subregions into convex polygons.

Remark 12.7. We will deform in such a way that the edges $\{v_1, v_2\}$ will maintain a length of at least 2. The proof that distances of at least 2 are maintained is given in Section 12.13.

We will deform in such a way that no vertex crosses a boundary of the subregion passing from the outside to the inside.

Edge length constraints prevent a vertex from crossing a boundary of the subregion from the inside to the outside. In fact, if v is to cross the edge $\{v_1, v_2\}$, the simplex $S = \{0, v_1, v, v_2\}$ attains volume 0. We may assume, by the argument of the proof of Lemma 12.4, that there are no vertices enclosed over S. Because we are assuming that the subregion is not a triangle, we may assume that $|v - v_1| > 2t_0$. We have $|v| \in [2, 2t_0]$. If v is to cross $\{v_1, v_2\}$, we may assume that the dihedral angles of S along $\{0, v_1\}$ and $\{0, v_2\}$ are acute. Under these constraints, by the explicit formulas of Section 8 of [Ha6], the vertex v cannot cross out of the subregion

$$\Delta(S) \geq \Delta(2t_0^2, 4, 4, 3.2^2, 4, 2t_0^2) > 0. \tag{12.2}$$

We say that a corner v_1 is *visible* from another v_2 if $\{v_1, v_2\}$ lies over the subregion. A deformation may make v_1 visible from v_2, making it a candidate for a new distinguished edge. If $|v_1 - v_2| \leq 3.2$, then as soon as the deformation brings them into visibility (obstructed until then by some v), inequality (12.2) shows that $|v_1 - v|, |v_2 - v| \leq 2t_0$. So v_1, v, v_2 are consecutive edges on the polygonal boundary, and $|v_1 - v_2| \geq 2\sqrt{4 - t_0^2} > \sqrt{8}$. By the distinguished edge conditions for special simplices, $\{v_1, v_2\}$ is too long to be distinguished. In other words, there can be no potentially distinguished edges hidden behind corners. They are always formed in full view.

12.8. *Some Deformations*

Definition 12.8. Consider three consecutive corners v_3, v_1, v_2 of a subcluster R such that the dihedral angle of R at v_1 is greater than π. We call such a corner *concave*. (If the angle is less than π, we call it *convex*.) Similarly, the angle of a subregion is said to be convex or concave depending on whether it is less than or greater than π.

Let $S = S(y_1, \ldots, y_6) = \{0, v_1, v_2, v_3\}$, $y_i = |v_i|$. Suppose that $y_6 > y_5$. Let $x_i = y_i^2$.

Lemma 12.9. *At a concave vertex*, $\partial \operatorname{vor}_0 / \partial x_5 > 0$ *and* $\partial \tau_0 / \partial x_5 < 0$.

Proof. As x_5 varies, $\operatorname{dih}_i(S) + \operatorname{dih}_i(R)$ is constant for $i = 1, 2, 3$. The part of formula (7.13) for vor_0 that depends on x_5 can be written

$$-B(y_1)\operatorname{dih}(S) - B(y_2)\operatorname{dih}_2(S) - B(y_3)\operatorname{dih}_3(S) - 4\delta_{\mathrm{oct}}(\operatorname{quo}(R_{135}) + \operatorname{quo}(R_{315})),$$

where $B(y_i) = A(y_i/2) + \varphi_0$, $R_{135} = R(y_1/2, b, t_0)$, $R_{315} = R(y_3/2, b, t_0)$, $b = \eta(y_1, y_3, y_5)$, and $A(h) = (1 - h/t_0)(\varphi(h, t_0) - \varphi_0)$. Set $u_{135} = u(x_1, x_3, x_5)$ and $\Delta_i = \partial\Delta/\partial x_i$. (The notation comes from Section 8 of [Ha6] and Section 7 of this issue.) We have

$$\frac{\partial \operatorname{quo}(R(a, b, c))}{\partial b} = \frac{-a(c^2 - b^2)^{3/2}}{3b(b^2 - a^2)^{1/2}} \leq 0$$

and $\partial b/\partial x_5 \ge 0$. Also, $u \ge 0$, $\Delta \ge 0$ (see Section 8 of [Ha6]). So it is enough to show

$$V_0(S) = u_{135}\Delta^{1/2}\frac{\partial}{\partial x_5}(B(y_1)\,\mathrm{dih}(S) + B(y_2)\,\mathrm{dih}_2(S) + B(y_3)\,\mathrm{dih}_3(S)) < 0.$$

By the explicit formulas of Section 8 of [Ha6], we have

$$V_0(S) = -B(y_1)y_1\Delta_6 + B(y_2)y_2u_{135} - B(y_3)y_3\Delta_4.$$

For τ_0, we replace B with $B - \zeta pt$. It is enough to show that

$$V_1(S) = -(B(y_1) - \zeta pt)y_1\Delta_6 + (B(y_2) - \zeta pt)y_2u_{135} - (B(y_3) - \zeta pt)y_3\Delta_4 < 0.$$

The lemma now follows from an interval calculation. We note that the polynomials V_i are linear in x_4, and x_6, and this may be used to reduce the dimension of the calculation. □

We give a second form of the lemma when the dihedral angle of R is less than π, that is, at a convex corner.

Lemma 12.10. *At a convex corner,* $\partial\,\mathrm{vor}_0/\partial x_5 < 0$ *and* $\partial\tau_0/\partial x_5 > 0$, *if* $y_1, y_2, y_3 \in [2, 2t_0]$, $\Delta \ge 0$, *and* (i) $y_4 \in [2\sqrt{2}, 3.2]$, $y_5, y_6 \in [2, 2t_0]$, *or* (ii) $y_4 \ge 3.2$, $y_5, y_6 \in [2, 3.2]$.

Proof. We adapt the proof of the previous lemma. Now $\mathrm{dih}_i(S) - \mathrm{dih}_i(R)$ is constant, for $i = 1, 2, 3$, so the signs change. vor_0 depends on x_5 through

$$\sum B(y_i)\,\mathrm{dih}_i(S) - 4\delta_{\mathrm{oct}}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})).$$

So it is enough to show that

$$V_0 - 4\delta_{\mathrm{oct}}\Delta^{1/2}u_{135}\frac{\partial}{\partial x_5}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})) < 0.$$

Similarly, for τ_0, it is enough to show that

$$V_1 - 4\delta_{\mathrm{oct}}\Delta^{1/2}u_{135}\frac{\partial}{\partial x_5}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})) < 0.$$

By an interval calculation[74]

$$\begin{aligned} -4\delta_{\mathrm{oct}}u_{135}\frac{\partial}{\partial x_5}(\mathrm{quo}(R_{135}) + \mathrm{quo}(R_{315})) &< 0.82, \qquad \text{on} \quad [2, 2t_0]^3,\\ &< 0.5, \qquad \text{on} \quad [2, 2t_0]^3, \quad y_5 \ge 2.189. \end{aligned}$$

The result now follows from the inequalities.[75] □

[74] CALC-984628285.
[75] CALC-984628285.

Return to the situation of concave corner v_1. Let v_2, v_3 be the adjacent corners. By increasing x_5, the vertex v_1 moves away from every corner w for which $\{v_1, w\}$ lies outside the region. This deformation then satisfies the constraint of Remark 12.7. Stretch the shorter of $\{v_1, v_2\}$, $\{v_1, v_3\}$ until $|v_1 - v_2| = |v_1 - v_3| = 3.07$ (or until a new distinguished edge forms, etc.). Do this at all concave corners.

By stopping at 3.07, we prevent a corner crossing an edge from the outside to the inside. Let w be a corner that threatens to cross a distinguished edge $\{v_1, v_2\}$ as a result of the motion at a nonconvex vertex. To say that the crossing of the edge is from the outside to the inside implies more precisely that the vertex being moved is an endpoint, say v_1, of the distinguished edge. At the moment of crossing the simplex $\{0, v_1, v_2, w\}$ degenerates to a planar arrangement, with the radial projection of w lying over the geodesic arc connecting the radial projections of v_1 and v_2. To see that the crossing cannot occur, it is enough to note that the volume of a simplex with opposite edges of lengths at most $2t_0$ and 3.07 and other edges at least 2 cannot be planar. The extreme case is

$$\Delta(2^2, 2^2, (2t_0)^2, 2^2, 2^2, 3.07^2) > 0.$$

If $|v_1| \geq 2.2$, we can continue the deformations even further. We stretch the shorter of $\{v_1, v_2\}$ and $\{v_1, v_3\}$ until $|v_1 - v_2| = |v_1 - v_3| = 3.2$ (or until a new distinguished edge forms, etc.). Do this at all concave corners v_1 for which $|v_1| \geq 2.2$. To see that corners cannot cross an edge from the outside to the inside, we argue as in the previous paragraph, but replacing 3.07 with 3.2. The extreme case becomes

$$\Delta(2.2^2, 2^2, (2t_0)^2, 2^2, 2^2, 3.2^2) > 0.$$

12.9. *Truncated Corner Cells*

Because of the arguments in Section 12.8, we may assume without loss of generality that we are working with a subregion with the following properties. If v is a concave vertex and w is not adjacent to v, and yet is visible from v, then $|v - w| \geq 3.2$. If v is a concave corner, then $|v - w| \geq 3.07$ for both adjacent corners w. If v is a concave corner and $|v| \geq 2.2$, then $|v - w| \geq 3.2$ for both adjacent corners w. These hypotheses will remain in force through to the end of Section 12.

Recall from Definition 12.8 that we call a spherical region *convex* if its interior angles are all less than π. The case where the subregion is a convex triangle will be treated in Section 13.8. Hence, we may also assume in Sections 12.9–12.12 that the subregion is not a convex triangle.

We construct a *corner cell* at each corner. It depends on a parameter $\lambda \in [1.6, 1.945]$. In all applications, we take $\lambda = 1.945 = 3.2 - t_0$, $\lambda = 1.815 = 3.07 - t_0$, or $\lambda = 1.6 = 3.2/2$.

To construct the cell around the corner v, place a triangle along $\{0, v\}$ with sides $|v|$, t_0, λ (with λ opposite the origin). Generate the solid of rotation around the axis $\{0, v\}$. Extend to a cone over 0. Slice the solid by the perpendicular bisector of $\{0, v\}$, retaining the part near 0. Intersect the solid with a ball of radius t_0. The cones over the two boundary edges of the subregion at v make two cuts in the solid. Remove the slice that lies outside the cone over the subcluster. What remains is the corner cell at v with parameter λ.

Corner cells at corners separated by a distance less than 2λ may overlap. We define a truncation of the corner cell that has the property that the *truncated corner cells* at adjacent corners do not overlap. Let $\{0, v_i, v_j\}^\perp$ denote the plane perpendicular to the plane $\{0, v_i, v_j\}$ passing through the origin and the circumcenter of $\{0, v_i, v_j\}$.

Let v_1, v_2, v_3 be consecutive corners of a subcluster. Take the corner cell with parameter λ at the corner v_2. Slice it by the planes $\{0, v_1, v_2\}^\perp$ and $\{0, v_2, v_3\}^\perp$, and retain the part along the edge $\{0, v_2\}$. This is the truncated corner cell (tcc). By construction tcc's at adjacent corners are separated by a plane $(0, \cdot, \cdot)^\perp$. Tcc's at nonadjacent corners do not overlap if the corners are $\geq 2\lambda$ apart. Tcc's will only be used in subregions satisfying this condition. It will be shown in Section 12.11 that tcc's lie in the cone over the subregion (for suitable λ).

12.10. *Formulas for Truncated Corner Cells*

We will assign a score to tcc's, in such a way that the score of the subcluster can be estimated from the scores of the corner cells.

We write C_0 for a tcc. We write C_0^{u} for the corresponding untruncated corner cell. (Although we call this the untruncated corner cell to distinguish it from the corner cell, it is still truncated in the sense that it lies in the ball at the origin of radius t_0. It is untruncated in the sense that it is not cut by the planes $(\cdots)^\perp$.)

For any solid body X, we define the *geometric* truncated function by

$$\mathrm{vor}_0^{\mathrm{g}}(X) = 4(-\delta_{\mathrm{oct}}\,\mathrm{vol}(X) + \mathrm{sol}(X)/3)$$

the counterpart for squander

$$\tau_0^{\mathrm{g}}(X) = \zeta pt\,\mathrm{sol}(X) - \mathrm{vor}_0^{\mathrm{g}}(X).$$

The solid angle is to be interpreted as the solid angle of the cone formed by all rays from the origin through nonzero points of X. We may apply these definitions to obtain formulas for $\mathrm{vor}_0^{\mathrm{g}}(C_0)$, and so forth.

The formula for the score of a tcc differs slightly according to the convexity of the corner. We start with a convex corner v, and let v_1, v, and v_2 be consecutive corners in the subregion.

Let $S = \{0, v, v_1, v_2\}$ be a simplex with $|v_1 - v_2| \geq 3.2$. The formula for the score of a tcc $C_0(S)$ simplifies if the face of C_0 cut by $\{0, v, v_1\}^\perp$ does not meet the face cut by $\{0, v, v_2\}^\perp$. We make that assumption in this subsection. Set $\chi_0(S) = \mathrm{vor}_0^{\mathrm{g}}(C_0(S))$. (The function χ_0 is unrelated to the function χ that was introduced in Definition 5.14 to measure the orientation of faces.)

$$\begin{aligned}
\psi &= \mathrm{arc}(y_1, t_0, \lambda), \qquad h = y_1/2,\\
R'_{126} &= R(y_1/2, \eta_{126}, y_1/(2\cos\psi)), \qquad R_{126} = R(y_1/2, \eta_{126}, t_0),\\
\mathrm{sol}'(y_1, y_2, y_6) &= +\,\mathrm{dih}(R'_{126})(1 - \cos\psi) - \mathrm{sol}(R'_{126}),
\end{aligned}$$

$$\begin{aligned}\chi_0(S) \;=\; & \mathrm{dih}(S)(1-\cos\psi)\varphi_0 \\ & -\; \mathrm{sol}'(y_1, y_2, y_6)\varphi_0 - \mathrm{sol}'(y_1, y_3, y_5)\varphi_0 \\ & +\; A(h)\,\mathrm{dih}(S) - 4\delta_{\mathrm{oct}}(\mathrm{quo}(R_{126}) + \mathrm{quo}(R_{135})).\end{aligned}$$

In the three lines giving the formula for χ_0, the first line represents the score of the cone before it is cut by the planes $\{0, v, v_i\}^{\perp}$ and the perpendicular bisector of $\{0, v\}$. The second line is the correction resulting from cutting the tcc along the planes $\{0, v, v_i\}^{\perp}$. The face of the Rogers simplex R'_{126} lies along the plane $\{0, v, v_1\}^{\perp}$. The third line is the correction from slicing the tcc with the perpendicular bisector of $\{0, v\}$. This last term is the same as the term appearing for a similar reason in the formula for vor_0 in formula (7.13). In this formula R is the usual Rogers simplex and $\mathrm{quo}(R_{ijk})$ is the quoin coming from a Rogers simplex along the face with edges (ijk).

The formula for the untruncated corner cell is obtained by setting "sol′" and "quo" to "0" in the expression for χ_0. Thus,

$$\mathrm{vor}^{\mathrm{g}}(C_0^{\mathrm{u}}) = \mathrm{dih}(S)[(1-\cos\psi)\varphi_0 + A(h)].$$

The formula depends only on λ, the dihedral angle, and the height $|v|$. We write $C_0^{\mathrm{u}} = C_0^{\mathrm{u}}(|v|, \mathrm{dih})$, and suppress λ from the notation. The dependence on $\mathrm{dih}(S)$ is linear:

$$\tau_0^{\mathrm{g}}(C_0^{\mathrm{u}}(|v|, \mathrm{dih})) = (\mathrm{dih}/\pi)\tau_0^{\mathrm{g}}(C_0^{\mathrm{u}}(|v|, \pi)).$$

The dependence of χ_0 on the fourth edge $y_4 = |v_1 - v_2|$ comes through a term proportional to $\mathrm{dih}(S)$. Since the dihedral angle is monotonic in y_4, so is χ_0. Thus, under the assumption that $|v_1 - v_2| \ge 3.2$, we obtain an upper bound on χ_0 at $y_4 = 3.2$. Our deformations will fix the lengths of the other five variables, and monotonicity gives us the sixth. Thus, the tcc's lead to an upper bound on $\mathrm{vor}_0^{\mathrm{g}}$ (and a lower bound on τ_0^{g}) that does not require interval arithmetic.

At a concave vertex, the formula is similar. Replace "$\mathrm{dih}(S)$" with "$(2\pi - \mathrm{dih}(S))$" in the given expression for χ_0. We add a superscript minus to the name of the function at concave vertices, to denote this modification: $\chi_0^-(C_0)$.

12.11. *Containment of Truncated Corner Cells*

The assumptions made at the beginning of Section 12.9 remain in force.

Lemma 12.11. *Let v be a concave vertex with $|v| \ge 2.2$. The tcc at v with parameter $\lambda = 1.945$ lies in the truncated V-cell over R.*

Proof. Consider a corner cell at v and a distinguished edge $\{v_1, v_2\}$ forming the boundary of the subregion. The corner cell with parameter $\lambda = 1.945$ is contained in a cone of arcradius $\theta = \mathrm{arc}(2, t_0, \lambda) < 1.21 < \pi/2$ (in terms of the function *arc* of Section 9.7). Take two corners w_1, w_2, visible from v, between which the given bounding edge appears. (We may have $w_i = v_i$.) The two visible edges, $\{v, w_i\}$, have length ≥ 3.2. (Recall that the distinguished edges at v have been deformed to length 3.2.) They have arc-length at least $\mathrm{arc}(2t_0, 2t_0, 3.2) > 1.38$. The segment of the distinguished edge $\{v_1, v_2\}$ visible from v has arc-length at most $\mathrm{arc}(2, 2, 3.2) < 1.86$.

We check that the corner cell cannot cross the visible portion of the edge $\{v_1, v_2\}$. Consider the spherical triangle formed by the edges $\{v, w_1\}, \{v, w_2\}$ (extended as needed) and the visible part of $\{v_1, v_2\}$. Let C be the radial projection of v and let AB be the radial projection of the visible part of $\{v_1, v_2\}$. Pivot A and B toward C until the edges AC and BC have arc-length 1.38. The perpendicular from C to AB has length at least

$$\arccos(\cos(1.38)/\cos(1.86/2)) > 1.21 > \theta.$$

This proves that the corner cell lies in the cone over the subregion. □

Lemma 12.12. *Let v be a concave vertex. The truncated corner cell at v with parameter $\lambda = 1.815$ lies in the truncated V-cell over R.*

Proof. The proof proceeds along the same lines as the previous lemma, with slightly different constants. Replace 1.945 with 1.815, 1.38 with 1.316, and 1.21 with 1.1. Replace 3.2 with 3.07 in contexts giving a lower bound to the length of an edge at v, and keep it at 3.2 in contexts calling for an upper bound on the length of a distinguished edge. The constant 1.86 remains unchanged. □

Lemma 12.13. *The truncated corner cells with parameter* 1.6 *in a subregion do not overlap.*

Proof. We may assume that the corners are not adjacent. If a nonadjacent corner w is visible from v, then $|w - v| \geq 3.2$, and an interior point intersection p is incompatible with the triangle inequality: $|p - v| \leq 1.6$, $|p - w| < 1.6$. If w is not visible, we have a chain $v = v_0, v_1, \ldots, v_r = w$ such that v_{i+1} is visible from v_i. Imagine a taut string inside the subregion extending from v to w. The radial projections of v_i are the corners of the string's path. The string bends in an angle greater than π at each v_i, so the angle at each intermediate v_i is greater than π. That is, they are concave. Thus, by our deformations $|v_i - v_{i+1}| \geq 3.07$. The string has arc-length at least $r\,\mathrm{arc}(2t_0, 2t_0, 3.07) > r(1.316)$. However, the corner cells lie in cones of arcradius $\mathrm{arc}(2, t_0, \lambda) < 1$. So $2(1.0) > r(1.316)$, or $r = 1$. Thus, w is visible from v. □

Lemma 12.14. *The corner cell for $\lambda \leq 1.815$ does not overlap the t_0-cone wedge around another corner w.*

Proof. We take $\lambda = 1.815$. As in the previous proof, if there is overlap along a chain, then

$$\mathrm{arc}(2, t_0, \lambda) + \mathrm{arc}(2, t_0, t_0) > r\,\mathrm{arc}(2t_0, 2t_0, 3.07),$$

and again $r = 1$. So each of the two vertices in question is visible from the other. However, overlap implies $|p - v| \leq 1.815$ and $|p - w| < t_0$, forcing the contradiction $|w - v| < 3.07$. □

Lemma 12.15. *The corner cell for $\lambda \le 1.945$ at a corner v satisfying $|v| \ge 2.2$ does not overlap the t_0-cone wedge around another corner w.*

Proof. We take $\lambda = 1.945$. As in the previous proof, if there is overlap along a chain, then

$$\mathrm{arc}(2, t_0, \lambda) + \mathrm{arc}(2, t_0, t_0) > r\,\mathrm{arc}(2t_0, 2t_0, 3.2),$$

and again $r = 1$. Then the result follows from

$$|w - v| \le |p - v| + |p - w| < 1.945 + t_0 = 3.2. \qquad \square$$

Definition 12.16. By a *penalty-free* score, we mean the part of the scoring bound that does not include any of the penalty terms. We sometimes call the full score, including the penalty terms, the *penalty-inclusive* score.

Lemma 12.4 was stated in the context of a subregion before deformation, but a cursory inspection of the proof shows that the geometric conditions required for the proof remain valid by our deformations. (This assumes that the subregion is not a triangle, which we assumed at the beginning of Section 12.9.) In more detail, there is a solid CP_0 contained in the ball of radius t_0 at the origin, and lying over the cone of the subregion P such that a bound on the penalty-free subcluster score is $\mathrm{vor}_0^{\mathrm{g}}(CP_0)$ and squander $\tau_0^{\mathrm{g}}(CP_0)$.

Let $\{y_1, \ldots, y_r\}$ be a decomposition of the subregion into disjoint regions whose union is X. Then if we let $CP_0(y_i)$ denote the intersection of $CP_0(y_i)$ with the cone over y_i, we can write

$$\tau_0^{\mathrm{g}}(CP_0) = \sum_i \tau_0^{\mathrm{g}}(CP_0(y_i)).$$

These lemmas allow us to express bounds on the score (and squander) of a subcluster as a sum of terms associated with individual (truncated) corner cells. By Lemmas 12.11–12.15, these objects do not overlap under suitable conditions. Moreover, by the interpretation of terms provided by Section 12.4, the cones over these objects do not overlap, when the objects themselves do not. In other words, under the various conditions, we can take the (truncated) corner cells to be among the sets $CP_0(y_i)$.

To work a typical example, we place a tcc with parameter $\lambda = 1.6$ at each concave corner. We place a t_0-cone wedge X_0 at each convex corner. The cone over each object lies in the cone over the subregion. By Lemmas 12.5 and 9.20 (see the proof), the t_0-cone wedge X_0 squanders a positive amount. The part P' of the subregion outside all tcc's and outside the t_0-cone wedges squanders

$$\mathrm{sol}(P')(\zeta pt - \varphi_0) > 0,$$

where $\mathrm{sol}(P')$ is the part of the solid angle of the subregion lying outside the tccs. Dropping these positive terms, we obtain a lower bound on the penalty-free squander:

$$\tau_0^{\mathrm{g}}(CP_0) \ge \sum_{C_0} \tau_0^{\mathrm{g}}(C_0).$$

There is one summand for each concave corner of the subregion. Other cases proceed similarly.

12.12. *Convexity*

Lemma 12.17. *There are at most two concave corners.*

Proof. Use the parameter $\lambda = 1.6$ and place a tcc C_0 at each concave corner v. Let $C_0^{\mathrm{u}}(|v|, \mathrm{dih})$ denote the corresponding untruncated cell. The formula of Section 12.10 gives

$$\tau_0^{\mathrm{g}}(C_0) = \tau_0^{\mathrm{g}}(C_0^{\mathrm{u}}(|v|, \mathrm{dih})) - \mathrm{sol}'(y_1, y_2, y_6)\varphi_0' - \mathrm{sol}'(y_1, y_3, y_5)\varphi_0',$$

where $\varphi_0' = \zeta pt - \varphi_0 < 0.6671$. (The conditions $y_5 \geq 3.07$ and $y_6 \geq 3.07$ force the faces along the these edges to have circumradius greater than t_0, and this causes the "quo" terms in the formula to be zero.)

By monotonicity in dih, a lower bound on $\tau_0^{\mathrm{g}}(C_0^{\mathrm{u}})$ is obtained at $\mathrm{dih} = \pi$. $\tau_0(C_0^{\mathrm{u}}(|v|, \pi))$ is an explicit monotone decreasing rational function of $|v| \in [2, 2t_0]$, which is minimized for $|v| = 2t_0$. We find

$$\tau_0(C_0^{\mathrm{u}}(|v|, \mathrm{dih})) \geq \tau_0(C_0^{\mathrm{u}}(2t_0, \pi)) > 0.32.$$

The term $\mathrm{sol}'(y_1, y_3, y_5)$ is maximized when $y_3 = 2t_0$, $y_5 = 3.07$, so that $\mathrm{sol}' < 0.017$. (This was checked with interval arithmetic in Mathematica.) Thus,

$$\tau_0(C_0(v)) \geq 0.32 - 2(0.017)\varphi_0' > 0.297.$$

If there are three or more concave corners, then the penalty-free corner cells squander at least 3(0.297). The penalty is at most $\pi_{\max}$ (Section 12.6). So the penalty-inclusive squander is more than $3(0.297) - \pi_{\max} > (4\pi\zeta - 8)\,pt$. □

Lemma 12.18. *There are no concave corners of height at most* 2.2.

Proof. Suppose there is a corner of height at most 2.2. Place an untruncated corner cell $C_0^{\mathrm{u}}(|v|, \mathrm{dih})$ with parameter $\lambda = 1.815$ at that corner and a t_0-cone wedge at every other corner. The subcluster squanders at least $\tau_0(C_0(|v|, \pi)) - \pi_{\max}$. This is an explicit monotone decreasing rational function of one variable. The penalty-inclusive squander is at least

$$\tau_0(C_0^{\mathrm{u}}(2t_0, \pi)) - \pi_{\max} > (4\pi\zeta - 8)\,pt. \qquad \square$$

By the assumptions at the beginning of Section 12.9, the lemma implies that each concave corner has distance at least 3.2 from every other visible corner.

As in the previous lemma, when $\lambda = 1.945$, a lower bound on what is squandered by the corner cell is obtained for $|v| = 2t_0$, $\mathrm{dih} = \pi$. The explicit formulas give penalty-free squander > 0.734. Two disjoint corner cells give penalty-inclusive squander $> (4\pi\zeta - 8)\,pt$. Suppose two at v_1, v_2 overlap. The lowest bound is obtained when $|v_1 - v_2| = 3.2$, the shortest distance possible.

We define a function $f(y_1, y_2)$ that measures what the union of the overlapping corner cells squander. Set $y_i = |v_i|$, $\ell = 3.2$, and

$$\begin{aligned}
\alpha_1 &= \mathrm{dih}(y_1, t_0, y_2, \lambda, \ell, \lambda),\\
\alpha_2 &= \mathrm{dih}(y_2, t_0, y_1, \lambda, \ell, \lambda),\\
\mathrm{sol} &= \mathrm{sol}(y_2, t_0, y_1, \lambda, \ell, \lambda),\\
\varphi_i &= \varphi(y_i/2, t_0), \qquad i = 1, 2,\\
\lambda &= 3.2 - t_0 = 1.945,\\
f(y_1, y_2) &= 2(\zeta pt - \varphi_0)\,\mathrm{sol} + 2\sum_1^2 \alpha_i(1 - y_i/(2t_0))(\varphi_0 - \varphi_i)\\
&\quad + \sum_1^2 \tau_0(C(y_i, \lambda, \pi - 2\alpha_i)).
\end{aligned}$$

An interval calculation[76] gives $f(y_1, y_2) > (4\pi\zeta - 8)\,pt + \pi_{\max}$, for $y_1, y_2 \in [2, 2t_0]$.

We conclude that there is at most one concave corner. Let v be such a corner. If we push v toward the origin, the solid angle is unchanged and vor_0 is increased. Following this by the deformation of Section 12.8, we maintain the constraints $|v - w| = 3.2$, for adjacent corners w, while moving v toward the origin. Eventually $|v| = 2.2$. This is impossible by Lemma 12.18.

We verify that this deformation preserves the constraint $|v - w| \geq 2$, for all corners w such that $\{v, w\}$ lies entirely outside the subregion. If fact, every corner is visible from v, so that the subregion is star convex at v. We leave the details to the reader.

We conclude that all subregions can be deformed into convex polygons.

12.13. *Proof that Distances Remain at Least* 2

Remark 12.19. In Section 12.7, to allow for more flexible deformations, we drop all constraints on the lengths of (undistinguished) edges $\{v_1, v_2\}$ that cross the boundary of the subregion. We deform in such a way that the edges $\{v_1, v_2\}$ will maintain a length of at least 2.

Recall that we say that a vertex of a subregion is *convex* if its angle is less than π, and otherwise that is *concave* (Definition 12.8). In general, if P is a subregion and p_1 and p_2 are two vertices of P, there is a minimal curve joining p_1 and p_2 inside P. This curve is a finite sequence $e_1, \ldots, e_r$ of spherical geodesics. We refer to this sequence as the *sequence of arcs* from p_1 to p_2. The endpoint of each spherical arc is a vertex of P. All endpoints except possibly p_1 and p_2 are nonconvex. These endpoints are the radial

[76] CALC-984628285.

projections of corners of P: $v_0, v_1, \dots, v_{r+1}$, with $p(v_0) = p_1$ and $p(v_{r+1}) = p_2$. The vertex p_1 is visible from p_2 if and only if $r = 1$.

Lemma 12.20. *This deformation of a subregion at a concave corner v maintains a distance of at least 2 to every other corner w.*

Proof. The proof is by contradiction. We may assume that $|v - w| < \sqrt{8}$. We may assume that v and w are the first corners to violate the condition of being at least 2 apart, so that distances between other pairs of corners are at least 2. A distinguished edge connects v and w, if w is visible from v. So assume that w is not visible. Let $e(v_1, v_2)$ be the first distinguished edge crossed by the geodesic arc g from $p(v)$ to $p(w)$. Let p_0 be the intersection of $e(v_1, v_2)$ and g. By construction, the deformation moves v into the subregion, and the subregion P is concave at the corner v, so that the arc from $p(v)$ to $p(w)$ begins in P, then crosses out at $e(v_1, v_2)$.

Geometric considerations show that $|v_1 - v_2| \ge 2.91$. In fact, geometric considerations show that the shortest possible distance for $|v_1 - v_2|$ under the condition that $|v - w| \le 2$ is the length of the segment passing through the triangle of sides $2, 2t_0, 2t_0$ with both endpoints at distance exactly 2 from all three vertices of the triangle. This distance is greater than 2.91.

Let $e_1, \dots, e_r$ be the sequence of arcs from $p(v)$ to $p(v_1)$, and let $f_1, \dots, f_s$ be the sequence of arcs from $p(v)$ to $p(v_2)$. Since this sequence forms a minimal curve, the sum of the lengths of e_i is at most the sum of the lengths of $e(v, p_0)$ and $e(p_0, v_1)$, and the sum of the lengths of f_i is at most the sum of the lengths of $e(v, p_0)$ and $e(p_0, v_2)$.

Note that if $r + s \le 4$, then one of the edge-lengths must be at least 3.2, for otherwise the sequence of arcs are all distinguished or diagonals of specials, and this would not permit the existence of a corner w. That is, we can fully enumerate the corners of the subregion, and each projects radially to an endpoint in the sequence of arcs, or is a vertex of a special simplex. None of these corners is separated from v by the plane $\{0, v_1, v_2\}$.

We have $r + s \le 3$ by the following calculations; here $y \in [2, 2t_0]$:

$$\begin{aligned} 5\,\mathrm{arc}(2t_0, 2t_0, 2) &> \mathrm{arc}(2, 2, 3.2) + 2\,\mathrm{arc}(2, 2, 2),\\ 3\,\mathrm{arc}(2t_0, 2t_0, 2) + \mathrm{arc}(2t_0, y, 3.2) &> \mathrm{arc}(y, 2, 3.2) + 2\,\mathrm{arc}(2, 2, 2),\\ 3\,\mathrm{arc}(2t_0, 2t_0, 2) + \mathrm{arc}(2t_0, y, 3.2) &> \mathrm{arc}(2, 2, 3.2) + 2\,\mathrm{arc}(y, 2, 2). \end{aligned}$$

First we prove the lemma in the special case that the distance from v to one of the endpoints, say v_1, of $\{v_1, v_2\}$ is at least 3.2. In this special case we claim that the constraints on the edge-lengths creates an impossible geometric configuration. The constraints are as follows. There are five points: $0, v_1, w, v, v_2$. The plane $\{0, v_1, v_2\}$ separates point w from v. The distance constraints are as follows:

$$2 \le |u| \le 2t_0,$$

for $u = v_1, w, v, v_2$, $|v - v_1| \ge 3.2$, $|v - w| \le 2$, $|v - v_2| \ge 2$, $|w - v_1| \ge 2$, $|w - v_2| \ge 2$, and $2 \le |v_1 - v_2| \le 3.2$.

If the segment $\{v, w\}$ passes through the triangle $\{0, v_1, v_2\}$, then the desired impossibility proof follows by geometric considerations. Again, if the segment $\{v_1, v_2\}$ passes through the triangle $\{0, v, w\}$, then the desired impossibility proof follows by geometric considerations, provided that $\{0, v_1, v_2, w\}$ are not coplanar. Assume for a contradiction that $\{0, v_1, v_2, w\}$ lie in the plane P. We move back to the nonplanar case if $|v_2 - v|$ is not 2 (pivot v_2 around $\{0, w\}$ toward v), if $|v_1 - v|$ is not 3.2 (pivot v_1 around $\{0, w\}$ toward v), if $|w - v|$ is not 2 (pivot w around $\{v_1, v_2\}$ away from v), or v is not $2t_0$ (pivot v and w simultaneously preserving $|w - v|$ around $\{v_1, v_2\}$). Therefore, we may assume without loss of generality that $|v_2 - v| = 2$, $|v_1 - v| = 3.2$, $|w - v| = 2$, and $|v| = 2t_0$.

Let p be the orthogonal projection of v to the plane P. Let $h = |v - p|$. The distances from p to $u \in P$ is $f(|v-u|, h) = \sqrt{|v - u|^2 - h^2}$. We consider two cases depending on whether we can find a line in P through p dividing the plane into a half-plane containing v_1, 0, and v_2, or into a half-plane containing v_1, w, and v_2. In the first case we have

$$\begin{aligned} 0 &= \operatorname{arc}(|p - v_1|, |p|, |v_1|) + \operatorname{arc}(|p - v_2|, |p|, |v_2|) \\ &\quad - \operatorname{arc}(|p - v_1|, |p - v_2|, |v_1 - v_2|) \\ &\geq \operatorname{arc}(f(3.2, h), f(2t_0, h), 2) + \operatorname{arc}(f(2, h), f(2t_0, h), 2) \\ &\quad - \operatorname{arc}(f(3.2, h), f(2, h), 3.2). \end{aligned} \tag{12.3}$$

The function arc is monotonic in the arguments and from this it follows easily that this function of h is positive on its domain $0 \leq h \leq \sqrt{3}$. This is a contradiction. (The upper bound $\sqrt{3}$ is determined by the condition that the triangle $\{w, v_1, v\}$, which is equilateral in the extreme case, exists under the given edge constraints.) In the second case, we obtain the related contradiction

$$\begin{aligned} 0 &= \operatorname{arc}(|p - v_1|, |p - w|, |v_1 - w|) + \operatorname{arc}(|p - v_2|, |p - w|, |v_2 - w|) \\ &\quad - \operatorname{arc}(|p - v_1|, |p - v_2|, |v_1 - v_2|) \\ &\geq \operatorname{arc}(f(3.2, h), f(2, h), 2) + \operatorname{arc}(f(2, h), f(2, h), 2) \\ &\quad - \operatorname{arc}(f(3.2, h), f(2, h), 3.2) \\ &> 0. \end{aligned} \tag{12.4}$$

Now assume that the distances from v to the vertices v_1 and v_2 are at most 3.2.

If $r + s = 2$, then v_1 and v_2 are visible from v. Thus, they are distinguished or diagonals of special simplices. As $\{v_1, v_2\}$ is also distinguished, the corners of P are fully enumerated: v, v_1, v_2, and the vertices of special simplices. Since none of these are w, we conclude that w does not exist in this case.

If $r+s = 3$, then say $r = 1$ and $s = 2$. We have $\{v, v_1\}$ is distinguished or the diagonal of a special simplex. Let $p(v)$, $p(u)$ be the endpoints of f_1, for some corner u. We have $|u - v_1| \geq \sqrt{8}$ because $\{u, v_1\}$ is not distinguished, and $\max(|u - v|, |u - v_1|) \geq 3.2$, because otherwise we enumerate all vertices of P as in the case $r + s = 2$, and find that w is not among them. However, now geometric considerations lead to a contradiction: there does not exist a configuration of five points 0, u, v, v_1, v_2, with all distances at least 2 satisfying these constraints. (This can be readily solved by geometric considerations.) □

13. Convex Polygons

13.1. *Deformations*

We divide the bounding edges over the polygon according to length $[2, 2t_0]$, $[2t_0, 2\sqrt{2}]$, $[2\sqrt{2}, 3.2]$. The deformations of Section 12.8 contract edges to the lower bound of the intervals (2, $2t_0$, or $2\sqrt{2}$) unless a new distinguished edge is formed. By deforming the polygon, we assume that the bounding edges have length 2, $2t_0$, or $2\sqrt{2}$. (There are a few instances of triangles or quadrilaterals that do not satisfy the hypotheses needed for the deformations. These instances are treated in Sections 13.8 and 13.9.)

Lemma 13.1. *Let $S = S(y_1, \ldots, y_6)$ be a simplex, with $x_i = y_i^2$, as usual. Let $y_4 \geq 2$, $\Delta \geq 0$, $y_5, y_6 \in \{2, 2t_0, 2\sqrt{2}\}$. Fixing all the variables but x_1, let $f(x_1)$ be one of the functions* $\text{s-vor}_0(S)$ *or* $-\tau_0(S)$. *We have $f''(x_1) > 0$ whenever $f'(x_1) = 0$.*

Proof. This is an interval calculation.[77] □

The lemma implies that f does not have an interior point local maximum for $x_1 \in [2^2, 2t_0^2]$. Fix three consecutive corners, v_0, v_1, v_2 of the convex polygon, and apply the lemma to the variable $x_1 = |v_1|^2$ of the simplex $S = \{0, v_0, v_1, v_2\}$. We deform the simplex, increasing f. If the deformation produces $\Delta(S) = 0$, then some dihedral angle is π, and the arguments for nonconvex regions bring us eventually back to the convex situation. Eventually y_1 is 2 or $2t_0$. Applying the lemma at each corner, we may assume that the height of every corner is 2 or $2t_0$. (There are a few cases where the hypotheses of the lemma are not met, and these are discussed in Sections 13.8 and 13.9.)

Lemma 13.2. *The convex polygon has at most seven sides.*

Proof. Since the polygon is convex, its perimeter on the unit sphere is at most a great circle 2π. If there are eight sides, the perimeter is at least $8\,\text{arc}(2t_0, 2t_0, 2) > 2\pi$. □

13.2. *Truncated Corner Cells*

The following lemma justifies using tcc's at the corners as an upper bound on the score (and a lower bound on what is squandered). We fix the truncation parameter at $\lambda = 1.6$.

Lemma 13.3. *Take a convex subregion that is not a triangle. Assume edges between adjacent corners have lengths $\in \{2, 2t_0, 2\sqrt{2}, 3.2\}$. Assume nonadjacent corners are separated by distances ≥ 3.2. Then the truncated corner cell at each vertex lies in the cone over the subregion.*

[77] CALC-311189443.

Proof. Place a tcc at v_1. For a contradiction, let $\{v_2, v_3\}$ be an edge that the tcc overlaps. Assume first that $|v_1 - v_i| \geq 2t_0$, $i = 2, 3$. Pivot so that $|v_1 - v_2| = |v_1 - v_3| = 2t_0$. Write $S(y_1, \ldots, y_6) = \{0, v_1, v_2, v_3\}$. Set $\psi = \mathrm{arc}(y_1, t_0, 1.6)$. A calculation[78] gives $\beta_\psi(y_1, y_2, y_6) < \mathrm{dih}_2(S)$.

Now assume $|v_1 - v_2| < 2t_0$. By the hypotheses of the lemma, $|v_1 - v_2| = 2$. If $|v_1 - v_3| < 3.2$, then $\{0, v_1, v_2, v_3\}$ is triangular, contrary to hypothesis. So $|v_1 - v_3| \geq 3.2$. Pivot so that $|v_1 - v_3| = 3.2$. Then[79]

$$\beta_\psi(y_1, y_2, y_6) < \mathrm{dih}_2(S),$$

where $\psi = \mathrm{arc}(y_1, t_0, 1.6)$, provided $y_1 \in [2.2, 2t_0]$. Also, if $y_1 \in [2.2, 2t_0]$, then

$$\mathrm{arc}(y_1, t_0, 1.6) < \mathrm{arc}(y_1, y_2, y_6).$$

If $y_1 \leq 2.2$, then $\Delta_1 \geq 0$, so $\partial\, \mathrm{dih}_2 / \partial x_3 \leq 0$. Set $x_3 = 2t_0^2$. Also, $\Delta_6 \geq 0$, so $\partial\, \mathrm{dih}_2 / \partial x_4 \leq 0$. Set $x_4 = 3.2^2$.

Let c be a point of intersection of the plane $\{0, v_1, v_2\}^\perp$ with the circle at distance $\lambda = 1.6$ from v_1 on the sphere centered at the origin of radius t_0. The angle along $\{0, v_2\}$ between the planes $\{0, v_2, v_1\}$ and $\{0, v_2, c\}$ is

$$\mathrm{dih}(R(y_2/2, \eta_{126}, y_1/(2\cos\psi))).$$

This angle is less[80] than $\mathrm{dih}_2(S)$. Also, $\Delta_1 \geq 0$, $\partial\, \mathrm{dih}_3 / \partial x_2 \leq 0$, so set $x_2 = 2t_0^2$. Then $\Delta_5 < 0$, so $\mathrm{dih}_2 > \pi/2$. This means that $\{0, v_1, v_2\}^\perp$ separates the tcc from the edge $\{v_2, v_3\}$. □

13.3. *Analytic Continuation*

In this subsection we assume that $\lambda = 1.6$ and that the tcc under consideration lies at a convex vertex.

Assume that the face cut by $\{0, v, v_1\}^\perp$ meets the face cut by $\{0, v, v_2\}^\perp$. Let c_i be the point on the plane $\{0, v, v_i\}^\perp$ satisfying $|c_i - v| = 1.6$, $|c_i| = t_0$. (Pick the root within the wedge between v_1 and v_2.) The overlap of the two faces is represented in Fig. 13.1.

We let c_0 be the point of height t_0 on the intersection of the planes $\{0, v, v_1\}^\perp$ and $\{0, v, v_2\}^\perp$. We claim that c_0 lies over the truncated spherical region of the tcc, rather than the wedges of t_0-cones or the Rogers simplices along the faces $\{0, v, v_1\}$ and $\{0, v, v_2\}$. (This implies that c_0 cannot protrude beyond the corner cell as depicted in the second frame of the figure.) To see the claim, consider the tcc as a function of $y_4 = |v_1 - v_2|$. When y_4 is sufficiently large the claim is certainly true. Contract y_4 until $c_0 = c_0(y_4)$ meets the perpendicular bisector of $\{0, v\}$. Then c_0 is equidistant from 0, v, v_1 and v_2 so it is the circumcenter of $\{0, v, v_1, v_2\}$. It has distance t_0 from the origin, so the circumradius is t_0. This implies that $y_4 \leq 2t_0$.

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[78] CALC-193836552.
[79] CALC-193836552.
[80] CALC-193836552.

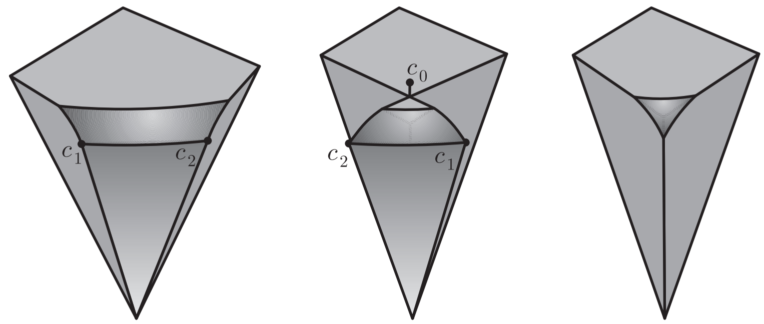

Fig. 13.1. Different forms of truncated corner cells are shown. The structure shown in the middle frame cannot occur.

The tcc is defined by the constraints represented in the third frame. The analytic continuation of the function $\chi_0(S) = \chi_0^{\mathrm{an}}(S)$, defined above, acquires a volume X, counted with a negative sign, lying under the spherical triangle (c_0, c_1, c_2). Extending our notation, we have an analytically defined function χ_0^{an} and a geometrically defined function χ_0^{g},

$$\begin{aligned} \chi_0^{\mathrm{an}}(S) &= \chi_0^{\mathrm{g}}(S) - \text{c-vor}_0(X), \qquad \text{where} \\ \text{c-vor}_0(X) &= 4(-\delta_{\mathrm{oct}}\,\mathrm{vol}(X) + \mathrm{sol}(X)/3) = \varphi_0\,\mathrm{sol}(X) < 0. \end{aligned}$$

So $\chi_0^{\mathrm{an}} > \chi_0^{\mathrm{g}}$, and we may always use $\chi_0(S) = \chi_0^{\mathrm{an}}(S)$ as an upper bound on the score of a tcc.

For example, with $\lambda = 1.6$ and $S = S(2.3, 2.3, 2.3, 2.9, 2, 2)$, we have

$$\chi_0^{\mathrm{an}}(S) \approx -0.103981, \qquad \chi_0^{\mathrm{g}}(S) \approx -0.105102,$$

or, if $S = S(2, 2, 2t_0, 3.2, 2, 2t_0)$, then

$$\chi_0^{\mathrm{an}}(S) \approx -0.0718957, \qquad \chi_0^{\mathrm{g}}(S) \approx -0.0726143.$$

13.4. *Penalties*

In Section 12.6 we determined the bound of $\pi_{\max} = 0.06688$ on penalties. In this section we give a more thorough treatment of penalties. Until now a penalty has been associated with a given standard region, but by taking the worst case on each subregion, we can move the penalties to the level of subregions. Roughly, each subregion should incur the penalties from the upright quarters that were erased along edges of that subregion. Each upright quarter of the original standard region is attached at an edge between adjacent corners of the standard cluster. The edges have lengths between 2 and $2t_0$. The deformations shrink the edges to length 2. We attach the penalty from the upright quarter to this edge of this subregion. In general, we divide the penalty evenly among the upright quarters along a common diagonal, without trying to determine a more detailed accounting. For example, the penalty 0.008 in Lemma 11.23 comes from three upright quarters. Thus, we give each of three edges a penalty of $0.008/3$, or, if there are only two upright quarters around the 3-unconfined upright diagonal, then each of the two upright quarters is assigned the penalty $0.00222/2$ (see Lemma 11.23).

The penalty $0.04683 = 3\xi_\Gamma$ in Section 12.6 comes from three upright quarters around a 3-crowded upright diagonal. Each of three edges is assigned a penalty of ξ_Γ. The penalty $0.03344 = 3\xi_\Gamma + \xi_{\kappa,\Gamma}$ comes from a 4-crowded upright diagonal of Section 11.7. It is divided among four edges. These are the only upright quarters that take a penalty when erased. (The case of two upright quarters over a flat quarter as in Lemma 11.3, are treated by a separate argument in Section 13.8. Loops are discussed in Section 13.12.)

The penalty can be reduced in various situations involving a masked flat quarter. For example, around a 3-crowded upright diagonal, if there is a masked flat quarter, two of the upright quarters are scored by the analytic function s-vor, so that the penalty plus adjustment is only[81,82] $0.034052 = 2\xi_V + \xi_\Gamma + 0.0114$. The adjustment 0.0114 reflects the scoring rules for masked flat quarters (Lemma 11.23). This we divide evenly among the three edges that carried the upright quarters. If e is an edge of the subregion R, let $\pi_0(R, e)$ denote the penalty and score adjustment along edge e of R.

In summary, we have the penalties,

$$\xi_\kappa,\ \xi_V,\ \xi_\Gamma,\ 0.008,$$

combined in various ways in the upright diagonals that are 3-unconfined, 3-crowded, or 4-crowded. There are score adjustments

$$0.0114 \quad \text{and} \quad 0.0063$$

from Section 11.9 for masked flat quarters. If the sum of these contributions is s, we set $\pi_0(R, e) = s/n$, for each edge e of R originating from an erased upright quarter of $\mathbf{S}_n^\pm$.

13.5. *Penalties and Bounds*

Recall that the bounds for flat quarters we wish to establish from Section 12.5 are $Z(3, 1) = 0.00005$ and $D(3, 1) = 0.06585$. Flat quarters arise in two different ways. Some flat quarters are present before the deformations begin. They are scored by the rules of Section 11.9. Others are formed by the deformations. In this case they are scored by vor_0. Since the flat quarter is broken away from the subregion as soon as the diagonal reaches $2\sqrt{2}$, and then is not deformed further, the diagonal is fixed at $2\sqrt{2}$. Such flat quarters can violate our desired inequalities. For example,

$$Z(3, 1) < \text{s-vor}_0(S(2, 2, 2, 2\sqrt{2}, 2, 2)) \approx 0.00898,$$

$$\tau_0(S(2, 2, 2, 2\sqrt{2}, 2, 2)) \approx 0.0593.$$

On the other hand, as we will see, the adjacent subregion satisfies the inequality by a comfortable margin. Therefore, we define a transfer ε from flat quarters to the adjacent

[81] CALC-73974037.
[82] CALC-764978100.

subregion. (In an exceptional region, the subregion next to a flat quarter along the diagonal is not a flat quarter.)

For a flat quarter Q, set

$$\varepsilon_\tau(Q) = \begin{cases} 0.0066 & \text{(deformation)}, \\ 0 & \text{(otherwise)}, \end{cases}$$

$$\varepsilon_\sigma(Q) = \begin{cases} 0.009 & \text{(deformation)}, \\ 0 & \text{(otherwise)}. \end{cases}$$

The nonzero value occurs when the flat quarter Q is obtained by deformation from an initial configuration in which Q is not a quarter. The value is zero when the flat quarter Q appears already in the undeformed standard cluster. Set

$$\begin{aligned} \pi_\tau(R) &= \sum_e \pi_0(R,e) + \sum_e \pi_0(Q,e) + \sum_Q \varepsilon_\tau(Q), \\ \pi_\sigma(R) &= \sum_e \pi_0(R,e) + \sum_e \pi_0(Q,e) + \sum_Q \varepsilon_\sigma(Q). \end{aligned}$$

The first sum runs over the edges of a subregion R. The second sum runs over the edges of the flat quarters Q that lie adjacent to R along the diagonal of Q.

The edges between corners of the polygon have lengths 2, $2t_0$, or $2\sqrt{2}$. Let k_0, k_1, and k_2 be the number of edges of these three lengths, respectively. By Lemma 13.2, we have $k_0 + k_1 + k_2 \le 7$. Let $\tilde\sigma$ denote any of the functions of (a)–(f) of Section 11.9. Let $\tilde\tau = \mathrm{sol}\,\zeta pt - \tilde\sigma$.

To prove Theorem 12.1, refining the strategy proposed in Section 12.5, we must show that for each flat quarter Q and each subregion R that is not a flat quarter, we have

$$\begin{aligned} \tilde\tau(Q) &> D(3,1) - \varepsilon_\tau(Q), \\ \tau_0(Q) &> D(3,1) - \varepsilon_\tau(Q), \qquad \text{if} \quad y_4(Q) = 2\sqrt{2}, \\ \tau_V(R) &> D(3,2) \qquad \text{(type } A\text{)}, \\ \tau_0(R) &> D(k_0+k_1+k_2, k_1+k_2) + \pi_\tau(R), \end{aligned} \tag{13.1}$$

where $D(n,k)$ is the function defined in Section 12.5. The first of these inequalities follows.[83–85] In general, we are given a subregion without explicit information about what the adjacent subregions are. Similarly, we have discarded all information about what upright quarters have been erased. Because of this, we assume the worst, and use the largest feasible values of π_τ.

Lemma 13.4. *We have* $\pi_\tau(R) \le 0.04683 + (k_0 + 2k_2 - 3)0.008/3 + 0.0066k_2$.

[83] CALC-193836552.
[84] CALC-148776243.
[85] CALC-163548682.

Proof. The worst penalty $0.04683 = 3\xi_\Gamma$ per edge comes from a 3-crowded upright diagonal. The number of penalized edges not on a simplex around a 3-crowded upright diagonal is at most $k_0 + 2k_2 - 3$. For every three edges, we might have one 3-unconfined upright diagonal. The other cases such as 4-crowded upright diagonals or situations with a masked flat quarter are readily seen to give smaller penalties. □

For bounds on the score, the situation is similar. The only penalties we need to consider are 0.008 from Lemma 11.23. If either of the other configurations of 3-crowded or 4-crowded upright diagonals occurs, then the score of the standard cluster is less than $s_8 = -0.228$, by Sections 11.6 and 11.7. This is the desired bound. So it is enough to consider subregions that do not have these upright configurations. Moreover, the penalty 0.008 does not occur in connection with masked flats. So we can take $\pi_\sigma(R)$ to be

$$(k_0 + 2k_2)0.008/3 + 0.009k_2.$$

If $k_0+2k_2 < 3$, we can strengthen this to $\pi_\sigma(R) = 0.009k_2$. Let $\tilde\sigma$ be any of the functions of (a)–(f) of Section 11.9. To prove Theorem 12.1, we will show

$$\begin{aligned}
\tilde\sigma(Q) &< Z(3,1) + \varepsilon_\sigma(Q),\\
\text{s-vor}_0(Q) &< Z(3,1) + \varepsilon_\sigma(Q), \qquad \text{if} \quad y_4(Q) = 2\sqrt{2},\\
\text{vor}_0(R) &< Z(3,2) \qquad (\text{type } A),\\
\text{vor}_0(R) &< Z(k_0+k_1+k_2, k_1+k_2) - \pi_\sigma(R).
\end{aligned} \tag{13.2}$$

The first of these inequalities follows.[86–88]

13.6. *Penalties*

Erasing an upright quarter of compression type gives a penalty of at most ξ_Γ and one of Voronoi type gives at most ξ_V. We take the worst possible penalty. It is at most $n\xi_\Gamma$ in an n-gon. If there is a masked flat quarter, the penalty is at most $2\xi_V$ from the two upright quarters along the flat quarter. We note in this connection that both edges of a polygon along a flat quarter lie on upright quarters, or neither does.

If an upright diagonal appears enclosed over a flat quarter, the flat quarter is part of a loop with context $(n, k) = (4, 1)$, for a penalty at most $2\xi'_\Gamma + \xi_V$. This is smaller than the bound on the penalty obtained from a loop with context $(n, k) = (4, 1)$, when the upright diagonal is not enclosed over the flat quarter:

$$\xi_\Gamma + 2\xi_V.$$

So we calculate the worst-case penalties under the assumption that the upright diagonals are not enclosed over flat quarters.

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[86] CALC-193836552.
[87] CALC-148776243.
[88] CALC-163548682.

A loop of context $(n, k) = (4, 1)$ gives $\xi_\Gamma + 2\xi_V$ or $3\xi_\Gamma$. A loop of context $(n, k) = (4, 2)$ gives $2\xi_\Gamma$ or $2\xi_V$.

If we erase a 3-unconfined upright diagonal, there is a penalty of 0.008 (or 0 if it masks a flat quarter). This is dominated by the penalty $3\xi_\Gamma$ of context $(n, k) = (4, 1)$.

Suppose we have an octagonal standard region. We claim that a loop does not occur in context $(n, k) = (4, 2)$. If there are at most three vertices that are not corners of the octagon, then there are at most twelve quasi-regular tetrahedra, and the score is at most

$$s_8 + 12\,pt < 8\,pt.$$

Assume there are more than three vertices that are not corners over the octagon. We squander

$$t_8 + \delta_{\text{loop}}(4, 2) + 4\tau_{\text{LP}}(5, 0) > (4\pi\zeta - 8)\,pt.$$

As a consequence, context $(n, k) = (4, 2)$ does not occur.

So there are at most two upright diagonals and at most six quarters, and the penalty is at most $6\xi_\Gamma$. Let f be the number of flat quarters This leads to

$$\pi_F = \begin{cases} 6\xi_\Gamma, & f = 0, 1, \\ 4\xi_\Gamma + 2\xi_V, & f = 2, \\ 2\xi_\Gamma + 4\xi_V, & f = 3, \\ 0, & f = 4. \end{cases}$$

The 0 is justified by a parity argument. Each upright quarter occurs in a pair at each masked flat quarter. However, there is an odd number of quarters along the upright diagonal, so no penalty at all can occur.

Suppose we have a heptagonal standard region. Three loops are a geometric impossibility. Assume there are at most two upright diagonals. If there is no context $(n, k) = (4, 2)$, then we have the following bounds on the penalty:

$$\pi_F = \begin{cases} 6\xi_\Gamma, & f = 0, \\ 4\xi_\Gamma + 2\xi_V, & f = 1, \\ 3\xi_\Gamma, & f = 2, \\ \xi_\Gamma + 2\xi_V, & f = 3. \end{cases}$$

If an upright diagonal has context $(n, k) = (4, 2)$, then

$$\pi_F = \begin{cases} 5\xi_\Gamma, & f = 0, 1, \\ 3\xi_\Gamma + 2\xi_V, & f = 2, \\ \xi_\Gamma + 4\xi_V, & f = 3. \end{cases}$$

This gives the bounds used in the diagrams of cases.

13.7. *Constants*

Theorem 12.1 now results from the calculation of a host of constants. Perhaps there are simpler ways to do it, but it was a routine matter to run through the long list of constants by computer. What must be checked is that the inequalities (13.1) and (13.2) of Section 13.5 hold for all possible convex subregions. Call these inequalities the D and Z inequalities. This section describes in detail the constants to check.

We begin with a subregion given as a convex n-gon, with at least four sides. The heights of the corners and the lengths of edges between adjacent edges have been reduced by deformation to a finite number of possibilities (lengths 2, $2t_0$, or lengths 2, $2t_0$, $2\sqrt{2}$, respectively). By Lemma 13.2, we may take $n = 4, 5, 6, 7$. Not all possible assignments of lengths correspond to a geometrically viable configuration. One constraint that eliminates many possibilities, especially heptagons, is that of Section 13.1: the perimeter of the convex polygon is at most a great circle. Eliminate all length-combinations that do not satisfy this condition. When there is a special simplex it can be broken from the subregion and scored[89] separately unless the two heights along the diagonal are 2. We assume in all that follows that all specials that can be broken off have been. There is a second condition related to special simplices. We have $\Delta(2t_0^2, 2^2, 2^2, x^2, 2^2, 2^2) < 0$, if $x > 3.114467$. This means that if the cluster edges along the polygon are $(y_1, y_2, y_3, y_5, y_6) = (2t_0, 2, 2, 2, 2)$, the simplex must be special ($y_4 \in [2\sqrt{2}, 3.2]$).

The easiest cases to check are those with no special simplices over the polygon. In other words, these are subregions for which the distances between nonadjacent corners are at least 3.2. In this case we approximate the score (and what is squandered) by tcc's at the corners. We use monotonicity to bring the fourth edge to length 3.2. We calculate the tcc constant bounding the score, checking that it is less than the constant $Z(k_0 + k_1 + k_2, k_1 + k_2) - \pi_\sigma$, from the Z inequalities. The D inequalities are verified in the same way.

When $n = 5, 6, 7$, and there is one special simplex, the situation is not much more difficult. By our deformations, we decrease the lengths of edges 2, 3, 5, 6 of the special to 2. We remove the special by cutting along its fourth edge e (the diagonal). We score the special with weak bounds.[90] Along the edge e, we then apply deformations to the $(n-1)$-gon that remains. If this deformation brings e to length $2\sqrt{2}$, then the $(n-1)$-gon may be scored with tcc's as in the previous paragraph. However there are other possibilities. Before e drops to $2\sqrt{2}$, a new distinguished edge of length 3.2 may form between two corners (one of the corners will be a chosen endpoint of e). The subregion breaks in two. By deformations, we eventually arrive at $e = 2\sqrt{2}$ and a subregion with diagonals of length at least 3.2. (There is one case that may fail to be deformable to $e = 2\sqrt{2}$, a pentagonal cases discussed further in Section 13.10.) The process terminates because the number of sides to the polygon drops at every step. A simple recursive computer procedure runs through all possible ways the subregion might break into pieces and checks that the tcc-bound gives the D and Z inequalities. The same argument works if there is a special simplex that overlaps each of the other special simplices in the subcluster.

When $n = 6, 7$ and there are two nonoverlapping special simplices, a similar argument can be applied. Remove both specials by cutting along the diagonals. Then deform both diagonals to length $2\sqrt{2}$, taking into account the possible ways that the subregion can break into pieces in the process. In every case the D and Z inequalities are satisfied.

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[89] CALC-148776243.
[90] CALC-148776243.

There are a number of situations that arise that escape this generic argument and were analyzed individually. These include the cases involving more than two special simplices over a given subregion, two special simplices over a pentagon, or a special simplex over a quadrilateral. Also, the deformation lemmas are insufficient to bring all of the edges between adjacent corners to one of the three standard lengths $2, 2t_0, 2\sqrt{2}$ for certain triangular and quadrilateral regions. These are treated individually.

The next few sections describe the cases treated individually. The cases not mentioned in the sections that follow fall within the generic procedure just described.

13.8. *Triangles*

With triangular subregions there is no need to use any of the deformation arguments because the dimension is already sufficiently small to apply interval arithmetic directly to obtain our bounds. There is no need for the tcc-bound approximations.

Flat quarters and simplices of type A are treated by a computer calculation.[91] Other simplices are scored by the truncated function s-vor_0. We break the edges between corners into the cases $[2, 2t_0)$, $[2t_0, 2\sqrt{2})$, and $[2\sqrt{2}, 3.2]$. Let k_0, k_1, and k_2, with $k_0+k_1+k_2 = 3$, be the number of edges in the respective intervals.

If $k_2 = 0$, we can improve the penalties,

$$\pi_\tau = \pi_\sigma = 0.$$

To see this, first we observe that there can be no 3-crowded or 4-crowded upright diagonals. By placing three or more quarters around an upright diagonal, if the subregion is triangular, the upright diagonal becomes surrounded by anchored simplices, a case deferred until Section 13.12.

If $k_0 = k_1 = k_2 = 1$, we can take $\pi'_\tau = \xi_\Gamma + 2\xi_V + 0.0114 = 0.034052$. A few cases are needed to justify this constant. If there are no 3-crowded upright diagonals, π'_τ is at most

$$[\xi_\Gamma + 2\xi_V + \xi_{\kappa,\Gamma}]3/4 < 0.0254,$$

or

$$[\xi_\Gamma + 2\xi_V + \xi_{\kappa,\Gamma}]2/4 + 0.008/3 < 0.0254$$

If there are at most two edges in the subregion coming from a 3-crowded upright diagonal, then

$$(\xi_\Gamma + 2\xi_V + 0.0114)2/3 + 0.008/3 < 0.0254.$$

If three edges come from the simplices of a 3-crowded upright diagonal, we get 0.034052. To get somewhat sharper bounds, we consider how the edge k_2 was formed. If it is obtained by deformation from an edge in the standard region of length ≥ 3.2, then it becomes a distinguished edge when the length drops to 3.2. If the edge in the standard region already has length ≤ 3.2, then it is distinguished before the deformation process

[91] CALC-163548682.

begins, so that the subregion can be treated in isolation from the other subregions. We conclude that when $\pi'_\tau = 0.034052$ we can take $y_4 \geq 2.6$ or $y_5 = 3.2$ (Remark 11.22).

The D and Z inequalities now follow.[92,93]

13.9. *Quadrilaterals*

We introduce some notation for the heights and edge lengths of a convex polygon. The heights will generally be 2 or $2t_0$, the edge lengths between consecutive corners will generally be 2, $2t_0$, or $2\sqrt{2}$. We represent the edge lengths by a vector

$$(a_1, b_1, a_2, b_2, \ldots, a_n, b_n),$$

if the corners of an n-gon, ordered cyclically have heights a_i and if the edge length between corner i and $i+1$ is b_i. We say two vectors are equivalent if they are related by a different cyclic ordering on the corners of the polygon, that is, by the action of the dihedral group.

The vector of a polygon with a special simplex is equivalent to one of the form

$$(2, 2, a_2, 2, 2, \ldots).$$

If $a_2 = 2t_0$, then what we have is necessarily special (Section 13.7). However, if $a_2 = 2$, it is possible for the edge opposite a_2 to have length greater than 3.2.

Turning to quadrilateral regions, we use tcc scoring if both diagonals are greater than 3.2. Suppose that both diagonals are between $[2\sqrt{2}, 3.2]$, creating a pair of overlapping special simplices. The deformation lemma requires a diagonal longer than 3.2, so although we can bring the quadrilateral to the form

$$(a_1, 2, 2, 2, 2, 2, a_4, b_4),$$

the edges a_1, a_4, b_4 and the diagonal vary[94] continuously. We have bounds[95] on the score

$$\begin{aligned} \tau_0 &> 0.235, & \mathrm{vor}_0 &< -0.075, & \text{if} \quad b_4 &\in [2t_0, 2\sqrt{2}], \\ \tau_0 &> 0.3109, & \mathrm{vor}_0 &< -0.137, & \text{if} \quad b_4 &\in [2\sqrt{2}, 3.2]. \end{aligned}$$

We have $D(4,1) = 0.2052$, $Z(4,1) = -0.05705$. When $b_4 \in [2t_0, 2\sqrt{2}]$, we can take $\pi_\tau = \pi_\sigma = 0$. (We are excluding loops here.) When $b_4 \in [2\sqrt{2}, 3.2]$, we can take

$$\begin{aligned} \pi_\tau &= \pi_{\max} + 0.0066, \\ \pi_\sigma &= 0.008(5/3) + 0.009. \end{aligned}$$

It follows that the D and Z inequalities are satisfied.

[92] CALC-852270725.
[93] CALC-819209129.
[94] CALC-148776243.
[95] CALC-128523606.

Suppose that one diagonal has length $[2\sqrt{2}, 3.2]$ and the other has length at least 3.2. The quadrilateral is represented by the vector

$$(2, 2, a_2, 2, 2, b_3, a_4, b_4).$$

The hypotheses of the deformation lemma hold, so that $a_i \in \{2, 2t_0\}$ and $b_j \in \{2, 2t_0, 2\sqrt{2}\}$. To avoid quad clusters, we assume $b_4 \geq \max(b_3, 2t_0)$. These are one-dimensional with a diagonal of length $[2\sqrt{2}, 3.2]$ as the parameter. The required verifications[96] have been made by interval arithmetic.

13.10. *Pentagons*

Some extra comments are needed when there is a special simplex. The general argument outlined above removes the special, leaving a quadrilateral. The quadrilateral is deformed, bringing the edge that was the diagonal of the special to $2\sqrt{2}$. This section discusses how this argument might break down.

Suppose first that there is a special and that both diagonals on the resulting quadrilateral are at least 3.2. We can deform using either diagonal, keeping both diagonals at least 3.2. The argument breaks down if both diagonals drop to 3.2 before the edge of the special reaches $2\sqrt{2}$ and both diagonals of the quadrilateral lie on specials. When this happens, the quadrilateral has the form

$$(2, 2, 2, 2, 2, 2, 2, b_4),$$

where b_4 is the edge originally on the special simplex. If both diagonals are 3.2, this is rigid, with $b_4 = 3.12$. We find its score to be

$$\begin{aligned} \text{s-vor}_0(S(2, 2, 2, b_4, 3.2, 2)) + \text{s-vor}_0(S(2, 2, 2, 3.2, 2, 2)) + 0.0461 \ &< \ -0.205, \\ \tau_0(S(2, 2, 2, b_4, 3.2, 2)) + \tau_0(S(2, 2, 2, 3.2, 2, 2))2 \ &> \ 0.4645. \end{aligned}$$

So the D and Z inequalities hold easily.

If there is a special and there is a diagonal on the resulting quadrilateral ≤ 3.2, we have two nonoverlapping specials. It has the form

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, b_5).$$

The edges a_2 and a_4 lie on the special. If $b_5 > 2$, cut away one of the special simplices. What is left can be reduced to a triangle, or a quadrilateral case and then treated[97] by computer. Assume $b_5 = 2$. We have a pentagonal standard region. We may assume that there is no 3-crowded or 4-crowded upright diagonal, for otherwise Theorem 12.1 follows trivially from the bounds in Section 9. A pentagon can then have at most a 3-unconfined upright diagonal for a penalty of 0.008.

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[96] CALC-874876755.
[97] CALC-874876755.

If $a_2 = 2t_0$ or $a_4 = 2t_0$, we again remove a special simplex and produce triangles, quadrilaterals, or the special cases treated by computer.[98] We may impose the condition $a_2 = a_4 = b_5 = 2$. We score this full pentagonal arrangement by computer,[99] using the edge lengths of the two diagonals of the specials as variables. The inequalities follow.

13.11. *Hexagons and Heptagons*

We turn to hexagons. There may be three specials whose diagonals do not cross. Such a subcluster is represented by the vector

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, 2, a_6, 2).$$

The heights a_{2i} are 2 or $2t_0$. Draw the diagonals between corners 1, 3, and 5. This is a three-dimensional configuration, determined by the lengths of the three diagonals, which is treated by computer.[100]

There is one case with a special simplex that did not satisfy the generic computer-checked inequalities for what is to be squandered. Its vector is

$$(a_1, 2, 2, 2, 2, 2, 2, b_4, 2, 2, 2, 2),$$

with $a_1 = b_4 = 2t_0$. A vertex of the special simplex has height $a_1 = 2t_0$ and all other corners have height 2. The subregion is a hexagon with one edge longer than 2. We have $D(6, 1) = 0.48414$. This is certainly obtained if the subregion contains a 3-crowded upright diagonal, squandering 0.5606. However, if this configuration does not appear, we can decrease π_τ to $0.03344 + (2/3)0.008$, a constant coming from 4-crowded upright diagonals in Section 12.6. With this smaller penalty the inequality is satisfied.

Now turn to heptagons.The bound 2π on the perimeter of the polygon eliminates all but one equivalence class of vectors associated with a polygon that has two or more potentially specials simplices. The vector is

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, 2, a_6, 2, a_7, 2),$$

$a_2 = a_4 = a_6 = a_7 = 2t_0$. In other words, the edges between adjacent corners are 2 and four heights are $2t_0$. There are two specials. This case is treated by the procedure outlined for subregions with two specials whose diagonals do not cross.

13.12. *Loops*

We now return to a collection of anchored simplices that surround the upright diagonal. This is the last case needed to complete the proof of Theorem 12.1. There are four or

[98] CALC-874876755.
[99] CALC-692155251.
[100] CALC-692155251.

five anchored simplices around the upright diagonal. There are linear inequalities[101–106] satisfied by the anchored simplices, broken up according to type: upright, type C, opposite edge > 3.2, etc. The anchored simplices are related by the constraint that the sum of the dihedral angles around the upright diagonal is 2π. We run a linear program in each case based on these linear inequalities, subject to this constraint to obtain bounds on the score and what is squandered by the anchored simplices.

When the edge opposite the diagonal of an anchored simplex has length $\in [2\sqrt{2}, 3.2]$ and the simplex adjacent to the anchored simplex across that edge is a special simplex, we use inequalities[107,108] that run parallel to the similar system.[109,110] It is not necessary to run separate linear programs for these. It is enough to observe that the constants for what is squandered improve on those from the similar system[111] and that the constants for the score in one system[112] differ with those of the other[113] by no more than 0.009.

When the dihedral angle of an anchored simplex is greater than 2.46, the simplex is dropped, and the remaining anchored simplices are subject to the constraint that their dihedral angles sum to at most $2\pi - 2.46$. There cannot be an anchored simplex with dihedral angle greater than 2.46 when there are five anchors: $2.46 + 4(0.956) > 2\pi$. There cannot[114] be two anchored simplices with dihedral angle greater than 2.46: $2(2.46 + 0.956) > 2\pi$.

The following table summarizes the linear programming results:

(n, k)	$D_{LP}(n, k)$	$D(n, k)$	$Z_{LP}(n, k)$	$Z(n, k)$
(4, 0)	0.1362	0.1317	0	0
(4, 1)	0.208	0.20528	−0.0536	−0.05709
(4, 2)	0.3992	0.27886	−0.2	−0.11418
(4, 3)	0.6467	0.35244	−0.424	−0.17127
(5, 0)	0.3665	0.27113	−0.157	−0.05704
(5, 1)	0.5941	0.34471	−0.376	−0.11413
$(5, \geq 2)$	0.9706	$(4\pi\zeta - 8)\,pt$	$*$	$*$

The bound for $D(4, 0)$ comes from Lemma 10.8. A few more comments are needed for $Z(4, 1)$. Let $S = S(y_1, \ldots, y_6)$ be the anchored simplex that is not a quarter. If $y_4 \geq 2\sqrt{2}$ or $\mathrm{dih}(S) \geq 2.2$, the linear programming bound is $< Z(4, 1)$. With this, if $y_1 \leq 2.75$, we have[115] $\sigma(S) < Z(4, 1)$. However, if $y_1 \geq 2.75$, the three upright quarters

[101] CALC-815492935.
[102] CALC-729988292.
[103] CALC-531888597.
[104] CALC-628964355.
[105] CALC-934150983.
[106] CALC-187932932.
[107] CALC-485049042.
[108] CALC-209361863.
[109] CALC-531888597.
[110] CALC-628964355.
[111] CALC-531888597.
[112] CALC-485049042.
[113] CALC-531888597.
[114] CALC-83777706.
[115] CALC-855294746.

along the upright diagonal satisfy

$$\nu < -0.3429 + 0.24573\,\mathrm{dih}\,.$$

With this stronger inequality, the linear programming bound becomes $< Z(4, 1)$. This completes the proof of Theorem 12.1.

Lemma 13.5. *Consider an upright diagonal that is a loop. Let R be the standard region that contains the upright diagonal and its surrounding simplices. Then the following contexts (m, k) are the only ones possible. Moreover, the constants that appear in the columns marked σ and τ are upper and lower bounds respectively for $\tau_R(D)$ when R contains one loop of that context.*

$n = n(R)$	(m, k)	σ	τ
4			
	(4, 0)	−0.0536	0.1362
5			
	(4, 1)	s_5	0.27385
	(5, 0)	−0.157	0.3665
6			
	(4, 1)	s_6	0.41328
	(4, 2)	−0.1999	0.5309
	(5, 1)	−0.37595	0.65995
7			
	(4, 1)	s_7	0.55271
	(4, 2)	−0.25694	0.67033
8			
	(4, 1)	s_8	0.60722
	(4, 2)	−0.31398	0.72484

Proof. In context (m, k), and if $n = n(R)$, we have

$$\sigma_R(D) < s_n + \mathrm{Z_{LP}}(m, k) - Z(m, k), \qquad \tau_R(D) > t_n + \mathrm{D_{LP}}(m, k) - D(m, k).$$

The result follows. □

In the context $(n, k) = (4, 3)$, the standard region R must have at least seven sides, $n(R) \geq 7$. Then

$$\begin{aligned}\tau(D) &\geq t_7 + \delta_{\mathrm{loop}}(4, 3)\\ &> (4\pi\zeta - 8)\,pt.\end{aligned}$$

Thus, we may assume that this context does not occur.

If the context (5, 1) appears in an octagon, we have

$$\tau(D) > \delta_{\mathrm{loop}}(5, 1) + t_8 > (4\pi\zeta - 8)\,pt.$$

If this appears in a heptagon, we have

$$\tau(D) > \delta_{\mathrm{loop}}(5, 1) + t_7 + 0.55\,pt > (4\pi\zeta - 8)\,pt,$$

because there must be a vertex that is not a corner of the heptagon. It cannot appear on a pentagon.

14. Further Bounds in Exceptional Regions

14.1. *Small Dihedral Angles*

Recall that Section 12.1 defines an integer $n(R)$ that is equal to the number of sides if the region is a polygon. Recall that if the dihedral angle along an edge of a standard cluster is at most 1.32, then there is a flat quarter along that edge (Lemma 11.30).

Lemma 14.1. *Let R be an exceptional cluster with a dihedral angle ≤ 1.32 at a vertex v. Then R squanders $> t_n + 1.47\,pt$, where $n = n(R)$.*

Proof. In most cases we establish the stronger bound $t_n + 1.5\,pt$. In the proof of Theorem 12.1 we erase all upright diagonals, except those completely surrounded by anchored simplices. The contribution to t_n from the flat quarter Q at v in that proof is $D(3, 1)$ (Section 12.5 and inequalities (13.1)). Note that $\varepsilon_\tau(Q) = 0$ here because there are no deformations. If we replace $D(3, 1)$ with $3.07\,pt$ from Lemma 11.30, then we obtain the bound. Now suppose the upright diagonal is completely surrounded by anchored simplices. Analyzing the constants of Section 13.12, we see that $\mathrm{D_{LP}}(n, k) - D(n, k) > 1.5\,pt$ except when $(n, k) = (4, 1)$.

Here we have four anchored simplices around an upright diagonal. Three of them are quarters. We erase and take a penalty. Two possibilities arise. If the upright diagonal is enclosed over the flat quarter, its height is ≥ 2.6 by geometric considerations and the top face of the flat quarter has circumradius at least $\sqrt{2}$. The penalty is $2\xi'_\Gamma + \xi_V$, so the bound holds by the last statement of Lemma 11.30.

If, on the other hand, the upright diagonal is not enclosed over the flat diagonal, the penalty is $\xi_\Gamma + 2\xi_V$. In this case we obtain the weaker bound $1.47\,pt + t_n$:

$$3.07\,pt > D(3, 1) + 1.47\,pt + \xi_\Gamma + 2\xi_V. \qquad \square$$

Remark 14.2. If there are r nonadjacent vertices with dihedral angles ≤ 1.32, we find that R squanders $t_n + r(1.47)\,pt$.

In fact, in the proof of the lemma, each $D(3, 1)$ is replaced with $3.07\,pt$ from Lemma 11.30. The only questionable case occurs when two or more of the vertices are anchors of the same upright diagonal (a loop). Referring to Section 13.12, we have the following observations about various contexts:

- (4, 1) can mask only one flat quarter and it is treated in the lemma.
- (4, 2) can mask only one flat quarter and $\mathrm{D_{LP}}(4, 2) - D(4, 2) > 1.47\,pt$.
- (5, 0) can mask two flat quarters. Erase the five upright quarters, and take a penalty $4\xi_V + \xi_\Gamma$. We get

$$D(3, 2) + 2(3.07)\,pt > t_5 + 4\xi_V + \xi_\Gamma + 2(1.47)\,pt.$$

- (5, 1) can mask two flat quarters, and $\mathrm{D_{LP}}(5, 1) - D(5, 1) > 2(1.47)\,pt$.

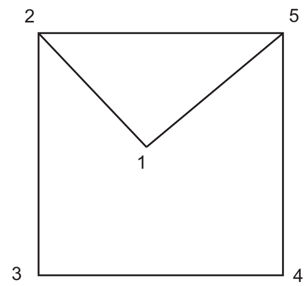

Fig. 14.1. A 4-circuit.

14.2. *A Particular* 4-*Circuit*

This subsection bounds the score of a particular 4-circuit on a contravening plane graph. The interior of the circuit consists of two faces: a triangle and a pentagon. The circuit and its enclosed vertex are show in Fig. 14.1 with vertices marked $p_1, \ldots, p_5$. The vertex p_1 is the enclosed vertex, the triangle is (p_1, p_2, p_5) and the pentagon is $(p_1, \ldots, p_5)$.

Suppose that D is a decomposition star whose associate graph contains such triangular and pentagonal standard regions. Recall that D determines a set $U(D)$ of vertices in Euclidean 3-space of distance at most $2t_0$ from the origin, and that each vertex p_i can be realized geometrically as a point on the unit sphere at the origin, obtained as the radial projection of some $v_i \in U(D)$.

Lemma 14.3. *One of the edges* $\{v_1, v_3\}$, $\{v_1, v_4\}$ *has length less than* $2\sqrt{2}$. *Both of the them have lengths less than* 3.02. *Also*, $|v_1| \geq 2.3$.

Proof. This is a standard exercise in geometric considerations as introduced in Section 4.2. (The reader should review that section for the framework of the following argument.) We deform the figure using pivots to a configuration $v_2, \ldots, v_5$ at height 2, and $|v_i - v_j| = 2t_0$, $(i, j) = (2, 3), (3, 4), (4, 5), (5, 2)$. We scale v_1 until $|v_1| = 2t_0$. We can also take the distance from v_1 to v_5 and to v_2 to be 2. If we have $|v_1 - v_3| \geq 2\sqrt{2}$, then we stretch the edge $|v_1 - v_4|$ until $|v_1 - v_3| = 2\sqrt{2}$. The resulting configuration is rigid. Pick coordinates to find that $|v_1 - v_4| < 2\sqrt{2}$. If we have $|v_1 - v_3| \geq 2t_0$, follow a similar procedure to reduce to the rigid configuration $|v_1 - v_3| = 2t_0$, to find that $|v_1 - v_4| < 3.02$. The estimate $|v_1| \geq 2.3$ is similar. □

There are restrictive bounds on the dihedral angles of the simplices $\{0, v_1, v_i, v_j\}$ along the edge $\{0, v_1\}$. The quasi-regular tetrahedron has a dihedral angle of at most[116] 1.875. The dihedral angles of the simplices $\{0, v_1, v_2, v_3\}$, $\{0, v_1, v_5, v_4\}$ adjacent to it are

[116] CALC-984463800.

at most[117] 1.63. The dihedral angle of the remaining simplex $\{0, v_1, v_3, v_4\}$ is at most[118] 1.51. This leads to lower bounds as well. The quasi-regular tetrahedron has a dihedral angle that is at least $2\pi - 2(1.63) - 1.51 > 1.51$. The dihedral angles adjacent to the quasi-regular tetrahedron is at least $2\pi - 1.63 - 1.51 - 1.875 > 1.26$. The remaining dihedral angle is at least $2\pi - 1.875 - 2(1.63) > 1.14$.

A decomposition star D determines a set of vertices $U(D)$ that are of distance at most $2t_0$ from the center of D. Three consecutive vertices p_1, p_2, and p_3 of a standard region are determined as the projections to the unit sphere of three corners v_1, v_2, and v_3, respectively in $U(D)$. By Lemma 11.30, if the interior angle of the standard region is less than 1.32, then $|v_1 - v_3| \leq \sqrt{8}$.

Lemma 14.4. *These two standard regions $F = \{R_1, R_2\}$ give $\tau_F(D) \geq 11.16\,pt$.*

Proof. Let dih denote the dihedral angle of a simplex along a given edge. Let S_{ij} be the simplex $\{0, v_1, v_i, v_j\}$, for $(i, j) = (2, 3), (3, 4), (4, 5), (2, 5)$. We have $\sum_{(4)} \operatorname{dih}(S_{ij}) = 2\pi$. Suppose one of the edges $\{v_1, v_3\}$ or $\{v_1, v_4\}$ has length $\geq 2\sqrt{2}$. Say $\{v_1, v_3\}$.

We have[119]

$$
\begin{aligned}
\tau(S_{25}) - 0.2529\operatorname{dih}(S_{25}) &> -0.3442,\\
\tau_0(S_{23}) - 0.2529\operatorname{dih}(S_{23}) &> -0.1787,\\
\hat{\tau}(S_{45}) - 0.2529\operatorname{dih}(S_{45}) &> -0.2137,\\
\tau_0(S_{34}) - 0.2529\operatorname{dih}(S_{34}) &> -0.1371.
\end{aligned}
$$

We have a penalty ξ_Γ for erasing, so that

$$
\begin{aligned}
\tau(D) &\geq \sum_{(4)} \tau_x(S_{ij}) - 5\xi_\Gamma\\
&> 2\pi(0.2529) - 0.3442 - 0.1787 - 0.2137 - 0.1371 - 5\xi_\Gamma\\
&> 11.16\,pt,
\end{aligned}
$$

where $\tau_x = \tau, \hat{\tau}, \tau_0$ as appropriate.

Now suppose $\{v_1, v_3\}$ and $\{v_1, v_4\}$ have length $\leq 2\sqrt{2}$. If there is an upright diagonal that is not enclosed over either flat quarter, the penalty is at most $3\xi_\Gamma + 2\xi_V$. Otherwise, the penalty is smaller: $4\xi'_\Gamma + \xi_V$. We have

$$
\begin{aligned}
\tau(D) &\geq \sum_{(4)} \tau(S_{ij}) - (3\xi_\Gamma + 2\xi_V)\\
&> 2\pi(0.2529) - 0.3442 - 2(0.2137) - 0.1371 - (3\xi_\Gamma + 2\xi_V)\\
&> 11.16\,pt.
\end{aligned}
$$

□

[117] CALC-821707685.
[118] CALC-115383627.
[119] CALC-572068135, CALC-723700608, CALC-560470084, and CALC-535502975.

14.3. *A Particular 5-Circuit*

Lemma 14.5. *Assume that R is a pentagonal standard region with an enclosed vertex v of height at most $2t_0$. Assume further that*:

- $|v_i| \le 2.168$ *for each of the five corners*.
- *Each interior angle of the pentagon is at most* 2.89.
- *If v_1, v_2, v_3 are consecutive corners over the pentagonal region*, *then*

$$|v_1 - v_2| + |v_2 - v_3| < 4.804.$$

- $\sum_5 |v_i - v_{i+1}| \le 11.407$.

Then $\sigma_R(D) < -0.2345$ or $\tau_R(D) > 0.6079$.

Proof. Since -0.4339 is less than this the lower bound, a 3-crowded upright diagonal does not occur. Similarly, since -0.25 is less than the lower bound, a 4-crowded upright diagonal does not occur (Lemma 11.18 and Definition 11.7).

Suppose that there is a loop in context $(n, k) = (4, 2)$. Again by Lemma 13.5 (with $n(R) = 7$),

$$\sigma_R(D) < -0.2345.$$

We conclude that all loops have context $(n, k) = (4, 1)$.

Case 1. *The vertex $v = v_{12}$ has distance at least $2t_0$ from the five corners of $U(D)$ over the pentagon*. The penalty to switch the pentagon to a pure vor_0 score is at most $5\xi_\Gamma$ (see Section 12.6). There cannot be two flat quarters because then

$$|v_{12}| > \mathcal{E}(S(2, 2, 2, 2t_0, 2\sqrt{2}, 2\sqrt{2}), 2t_0, 2t_0, 2t_0) > 2t_0.$$

Case 1*a*. Suppose there is one flat quarter, $|v_1 - v_4| \le 2\sqrt{2}$. There is a lower bound of 1.2 on the dihedral angles of the simplices $\{0, v_{12}, v_i, v_{i+1}\}$. This is obtained as follows. The proof relies on the convexity of the quadrilateral region. We leave it to the reader to verify that the following pivots can be made to preserve convexity. Disregard all vertices except $v_1, v_2, v_3, v_4, v_{12}$. We give the argument that $\mathrm{dih}(0, v_{12}, v_1, v_4) > 1.2$. The others are similar. Disregard the length $|v_1 - v_4|$. We show that

$$\begin{aligned} sd \;:=\; & \mathrm{dih}(0, v_{12}, v_1, v_2) + \mathrm{dih}(0, v_{12}, v_2, v_3) \\ & + \mathrm{dih}(0, v_{12}, v_3, v_4) < 2\pi - 1.2. \end{aligned}$$

Lift v_{12} so $|v_{12}| = 2t_0$. Maximize sd by taking $|v_1 - v_2| = |v_2 - v_3| = |v_3 - v_4| = 2t_0$. Fixing v_3 and v_4, pivot v_1 around $\{0, v_{12}\}$ toward v_4, dragging v_2 toward v_{12} until $|v_2 - v_{12}| = 2t_0$. Similarly, we obtain $|v_3 - v_{12}| = 2t_0$. We now have $sd \le 3(1.63) < 2\pi - 1.2$, by a calculation.[120]

[120] CALC-821707685.

Return to the original figure and move v_{12} without increasing $|v_{12}|$ until each simplex $\{0, v_{12}, v_i, v_{i+1}\}$ has an edge (v_{12}, v_j) of length $2t_0$. Interval calculations[121] show that the four simplices around v_{12} squander

$$2\pi(0.2529) - 3(0.1376) - 0.12 > (4\pi\zeta - 8)\,pt + 5\xi_\Gamma.$$

Case 1*b*. Assume there are no flat quarters. By hypothesis, the perimeter satisfies

$$\sum |v_i - v_{i+1}| \le 11.407.$$

We have $\operatorname{arc}(2, 2, x)'' = 2x/(16-x^2)^{3/2} > 0$. The arclength of the perimeter is therefore at most

$$2\operatorname{arc}(2, 2, 2t_0) + 2\operatorname{arc}(2, 2, 2) + \operatorname{arc}(2, 2, 2.387) < 2\pi.$$

There is a well-defined interior of the spherical pentagon, a component of area $< 2\pi$. If we deform by decreasing the perimeter, the component of area $< 2\pi$ does not get swapped with the other component.

Disregard all vertices but $v_1, \ldots, v_5, v_{12}$. If a vertex v_i satisfies $|v_i - v_{12}| > 2t_0$, deform v_i as in Section 12.8 until $|v_{i-1} - v_i| = |v_i - v_{i+1}| = 2$, or $|v_i - v_{12}| = 2t_0$. If at any time, four of the edges realize the bound $|v_i - v_{i+1}| = 2$, we have reached an impossible situation, because it leads to the contradiction[122]

$$2\pi = \sum^{(5)} \operatorname{dih} < 1.51 + 4(1.16) < 2\pi.$$

(This inequality relies on the observation, which we leave to the reader, that in any such assembly, pivots can by applied to bring $|v_{12} - v_i| = 2t_0$ for at least one edge of each of the five simplices.)

The vertex v_{12} may be moved without increasing $|v_{12}|$ so that eventually by these deformations (and reindexing if necessary) we have $|v_{12} - v_i| = 2t_0$, $i = 1, 3, 4$. (If we have $i = 1, 2, 3$, the two dihedral angles along $\{0, v_2\}$ satisfy[123] $< 2(1.51) < \pi$, so the deformations can continue.)

There are two cases. In both cases $|v_i - v_{12}| = 2t_0$, for $i = 1, 3, 4$.

(i) $|v_{12} - v_2| = |v_{12} - v_5| = 2t_0$.
(ii) $|v_{12} - v_2| = 2t_0$, $|v_4 - v_5| = |v_5 - v_1| = 2$.

Case (i) follows from interval calculations[124]

$$\sum \tau_0 \ge 2\pi(0.2529) - 5(0.1453) > 0.644 + 7\xi_\Gamma.$$

In case (ii) we have again

$$2\pi(0.2529) - 5(0.1453).$$

[121] CALC-467530297 and CALC-135427691.
[122] CALC-115383627 and CALC-603145528.
[123] CALC-115383627.
[124] CALC-312132053.

In this interval calculation we have assumed that $|v_{12} - v_5| < 3.488$. Otherwise, setting $S = (v_{12}, v_4, v_5, v_1)$, we have

$$\Delta(S) < \Delta(3.488^2, 4, 4, 8, (2t_0)^2, (2t_0)^2) < 0,$$

and the simplex does not exist. ($|v_4 - v_1| \geq 2\sqrt{2}$ because there are no flat quarters.) This completes Case 1.

Case 2: *The vertex* v_{12} *has distance at most* $2t_0$ *from the vertex* v_1 *and distance at least* $2t_0$ *from the others*. Let $\{0, v_{13}\}$ be the upright diagonal of a loop (4, 1). The vertices of the loop are not $\{v_2, v_3, v_4, v_5\}$ with v_{12} enclosed over $\{0, v_2, v_5, v_{13}\}$ by Lemma 11.5. The vertices of the loop are not $\{v_2, v_3, v_4, v_5\}$ with v_{12} enclosed over $\{0, v_1, v_2, v_5\}$ because this would lead to a contradiction:

$$y_{12} \geq \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 3.2), 2t_0, 2t_0, 2) > 2t_0$$

or

$$y_{12} \geq \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 3.2), 2, 2t_0, 2) > 2t_0.$$

We get a contradiction for the same reasons unless $\{v_1, v_{12}\}$ is an edge of some upright quarter of every loop of type (4, 1).

We consider two cases. (Case 2a) There is a flat quarter along an edge other than $\{v_1, v_{12}\}$. That is, the central vertex is v_2, v_3, v_4, or v_5. (Recall that the *central vertex* of a flat quarter is the vertex other than the origin that is not an endpoint of the diagonal.) (Case 2b) Every flat quarter has central vertex v_1.

Case 2*a*. We erase all upright quarters including those in loops, taking penalties as required. There cannot be two flat quarters by geometric considerations

$$\mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2\sqrt{2}, 2t_0), 2t_0, 2t_0, 2) > 2t_0,$$
$$\mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2\sqrt{2}, 2t_0), 2, 2t_0, 2t_0) > 2t_0.$$

The penalty is at most $7\xi_\Gamma$. We show that the region (with upright quarters erased) squanders $> 7\xi_\Gamma + 0.644$. We assume that the central vertex is v_2 (Case 2a(i)) or v_3 (Case 2a(ii)). In Case 2a(i), we have three types of simplices around v_{12}, characterized by the bounds on their edge lengths. Let $\{0, v_{12}, v_1, v_5\}$ have type A, $\{0, v_{12}, v_5, v_4\}$ and $\{0, v_{12}, v_4, v_3\}$ have type B, and let $\{0, v_{12}, v_3, v_1\}$ have type C. In Case 2a(ii) there are also three types. Let $\{0, v_{12}, v_1, v_2\}$ and $\{0, v_{12}, v_1, v_5\}$ have type A, $\{0, v_{12}, v_5, v_4\}$ type B, and $\{0, v_{12}, v_2, v_4\}$ type D. (There is no relation here between these types and the types of simplices A, B, and C defined in Section 9.) Upper bounds on the dihedral angles along the edge $\{0, v_{12}\}$ are given as calculations.[125] These upper bounds come as a result of a pivot argument similar to that establishing the bound 1.2 in Case 1a.

These upper bounds imply the following lower bounds. In Case 2a(i),

$$\begin{aligned} \text{dih} &> 1.33 \quad (\text{A}),\\ \text{dih} &> 1.21 \quad (\text{B}),\\ \text{dih} &> 1.63 \quad (\text{C}), \end{aligned}$$

[125] CALC-821707685, CALC-115383627, CALC-576221766, and CALC-122081309.

and in Case 2a(ii),

$$\begin{aligned} \text{dih} &> 1.37 \quad (A), \\ \text{dih} &> 1.25 \quad (B), \\ \text{dih} &> 1.51 \quad (D), \end{aligned}$$

In every case the dihedral angle is at least 1.21. In Case 2a(i), the inequalities give a lower bound on what is squandered by the four simplices around $\{0, v_{12}\}$. Again, we move v_{12} without decreasing the score until each simplex $\{0, v_{12}, v_i, v_{i+1}\}$ has an edge satisfying $|v_{12} - v_j| \leq 2t_0$. Interval calculations[126] give

$$\begin{aligned} \sum_{(4)} \tau_0 &> 2\pi(0.2529) - 0.2391 - 2(0.1376) - 0.266 \\ &> 0.808. \end{aligned}$$

In Case 2a(ii), we have[127]

$$\begin{aligned} \sum_{(4)} \tau_0 &> 2\pi(0.2529) - 2(0.2391) - 0.1376 - 0.12 \\ &> 0.853. \end{aligned}$$

So we squander more than $7\xi_\Gamma + 0.644$, as claimed.

Case 2b. We now assume that there are no flat quarters with central vertex $v_2, \ldots, v_5$. We claim that v_{12} is not enclosed over $\{0, v_1, v_2, v_3\}$ or $\{0, v_1, v_5, v_4\}$. In fact, if v_{12} is enclosed over $\{0, v_1, v_2, v_3\}$, then we reach the contradiction[128]

$$\begin{aligned} \pi &< \text{dih}(0, v_{12}, v_1, v_2) + \text{dih}(0, v_{12}, v_2, v_3) \\ &< 1.63 + 1.51 < \pi. \end{aligned}$$

We claim that v_{12} is not enclosed over $\{0, v_5, v_1, v_2\}$. Let $S_1 = \{0, v_{12}, v_1, v_2\}$ and $S_2 = \{0, v_{12}, v_1, v_5\}$. We have by hypothesis,

$$y_4(S_1) + y_4(S_2) = |v_1 - v_2| + |v_1 - v_5| < 4.804.$$

An interval calculation[129] gives

$$\begin{aligned} \sum_{(2)} \text{dih}(S_i) &\leq \sum_{(2)} (\text{dih}(S_i) + 0.5(0.4804/2 - y_4(S_i))) \\ &< \pi. \end{aligned}$$

So v_{12} is not enclosed over $\{0, v_1, v_2, v_5\}$.

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[126] CALC-644534985, CALC-467530297, and CALC-603910880.
[127] CALC-135427691.
[128] CALC-821707685 and CALC-115383627.
[129] CALC-69064028.

Erase all upright quarters, taking penalties as required. Replace all flat quarters with s-vor$_0$-scoring taking penalties as required. (Any flat quarter has v_1 as its central vertex.) We move v_{12} keeping $|v_{12}|$ fixed and not decreasing $|v_{12} - v_1|$. The only effect this has on the score comes through the quoins along $\{0, v_1, v_{12}\}$. Stretching $|v_{12} - v_1|$ shrinks the quoins and increases the score. (The sign of the derivative of the quoin with respect to the top edge is computed in the proof of Lemma 12.9.)

If we stretch $|v_{12} - v_1|$ to length $2t_0$, we are done by Case 1 and Case 2a. (If deformations produce a flat quarter, use Case 2a, otherwise use Case 1.) By the claims, we can eventually arrange (reindexing if necessary) so that

(i) $|v_{12} - v_3| = |v_{12} - v_4| = 2t_0$, or
(ii) $|v_{12} - v_3| = |v_{12} - v_5| = 2t_0$.

We combine this with the deformations of Section 12.8 so that in case (i) we may also assume that if $|v_5 - v_{12}| > 2t_0$, then $|v_4 - v_5| = |v_5 - v_1| = 2$ and that if $|v_2 - v_{12}| > 2t_0$, then $|v_1 - v_2| = |v_2 - v_3| = 2$. In case (ii) we may also assume that if $|v_4 - v_{12}| > 2t_0$, then $|v_3 - v_4| = |v_4 - v_5| = 2$ and that if $|v_2 - v_{12}| > 2t_0$, then $|v_1 - v_2| = |v_2 - v_3| = 2$.

Break the pentagon into subregions by cutting along the edges (v_{12}, v_i) that satisfy $|v_{12} - v_i| \leq 2t_0$. So for example in case (i), we cut along (v_{12}, v_3), (v_{12}, v_4), (v_{12}, v_1), and possibly along (v_{12}, v_2) and (v_{12}, v_5). This breaks the pentagon into triangular and quadrilateral regions.

In case (ii) if $|v_4 - v_{12}| > 2t_0$, then the argument used in Case 1 to show that $|v_4 - v_{12}| < 3.488$ applies here as well. In case (i) or (ii) if $|v_{12} - v_2| > 2t_0$, then for similar reasons, we may assume

$$\Delta(|v_{12} - v_2|^2, 4, 4, 8, (2t_0)^2, |v_{12} - v_1|^2) \geq 0.$$

This justifies the hypotheses for the calculations[130] that we use. We conclude that

$$\sum \tau_0 \geq 2\pi(0.2529) - 3(0.1453) - 2(0.2391) > 0.6749.$$

If the penalty is less than $0.067 = 0.6749 - 0.6079$, we are done.

We have ruled out the existence of all loops except $(4, 1)$. Note that a flat quarter with central vertex v_1 gives penalty at most 0.02 by Lemma 11.29. If there is at most one such flat quarter and at most one loop, we are done:

$$3\xi_\Gamma + 0.02 < 0.067.$$

Assume there are two loops of context $(n, k) = (4, 1)$. They both lie along the edge $\{v_1, v_{12}\}$, which precludes any unmasked flat quarters. If one of the upright diagonals has height $\geq$ 2.696, then the penalty is at most $3\xi_\Gamma + 3\xi_V < 0.067$. Assume both heights are at most 2.696. The total interior angle of the exceptional face at v_1 is at least four times the dihedral angle of one of the flat quarters along $\{0, v_1\}$, or 4(0.74) by an interval calculation.[131] This is contrary to the hypothesis of an interior angle < 2.89. This completes Case 2. This shows that heptagons with pentagonal hulls do not occur. □

[130] CALC-312132053 and CALC-644534985.
[131] CALC-751442360.

Lemma 14.6. *Let R be an exceptional standard region. Let V be a set of vertices of R. If $v \in V$, let p_v be the number of triangular regions at v and let q_v be the number of quadrilateral regions at v. Assume that V has the following properties*:

1. *No two vertices in V are adjacent.*
2. *No two vertices in V lie on a common quadrilateral.*
3. *If $v \in V$, then there are five standard regions at v.*
4. *If $v \in V$, then the corner over v is a central vertex of a flat quarter in the cone over R.*
5. *If $v \in V$, then $p_v \geq 3$. That is, at least three of the five standard regions at v are triangular.*
6. *If $R' \neq R$ is an exceptional region at v, and if R has interior angle at least* 1.32 *at v, then R' also has interior angle at least* 1.32 *at v.*
7. *If $(p_v, q_v) = (3, 1)$, then the internal angle at v of the exceptional region is at most* 1.32.

Define a: $\mathbb{N} \to \mathbb{R}$ by

$$a(n) = \begin{cases} 14.8, & n = 0, 1, 2, \\ 1.4, & n = 3, \\ 1.5, & n = 4, \\ 0, & \textit{otherwise}. \end{cases}$$

Let $\{F\}$ be the union of $\{R\}$ with the set of triangular and quadrilateral regions that have a vertex at some $v \in V$. Then

$$\sum_F \tau_F(D) > \sum_{v \in V} (p_v d(3) + q_v d(4) + a(p_v))\, pt.$$

Proof. We erase all upright diagonals in the Q-system, except for those that carry a penalty: loops, 3-unconfined, 3-crowded, and 4-crowded diagonals.

We assume that if $(p_v, q_v) = (3, 1)$, then the internal angle is at most 1.32. Because of this, if we score the flat quarter by vor_0, then the flat quarter Q satisfies (Lemma 11.30)

$$\mathrm{vor}_0(Q) > 3.07\, pt > 1.4\, pt + D(3, 1) + 2\xi_V + \xi_\Gamma. \tag{14.1}$$

Every flat quarter that is masked by a remaining upright quarter in the Q-system has $y_4 \geq 2.6$. Moreover, $y_1 \geq 2.2$ or $y_4 \geq 2.7$. Let $\pi_v = 2\xi_V + \xi_\Gamma$ if the flat quarter is masked, and $\pi_v = 0$ otherwise.

We claim that the flat quarter (scored by vor_0) together with the triangles and quadrilaterals at a given vertex v squander at least

$$(p_v d(3) + q_v d(4) + a(p_v))\, pt + D(3, 1) + \pi_v. \tag{14.2}$$

If $p_v = 4$, this is CALC-314974315. If $p_v = 3$, we may assume by the preceding remarks that there are two exceptional regions at v. If the internal angle of R at v is at most 1.32, then we use inequality (14.1). If the angle is at least 1.32, then by hypothesis, the angle R' at v is at least 1.32. We then appeal to the calculations CALC-675785884 and CALC-193592217.

To complete the proof of the lemma, it is enough to show that we can erase the upright quarters masking a flat quarter at v without incurring a penalty greater than π_v. For then, by summing the inequality (14.2) over v, we obtain the result.

If the upright diagonal is enclosed over the masked flat quarter, then the upright quarters can be erased with penalty at most ξ_V (by Remark 11.28). Assume the upright diagonal is not enclosed over the masked flat quarter.

If there are at most three upright quarters, the penalty is at most $2\xi_V + \xi_\Gamma$. Assume four or more upright quarters. If the upright diagonal is not a loop, then it must be 4-crowded. This can be erased with penalty

$$2\xi_V + 2\xi_\Gamma - \kappa < 2\xi_V + \xi_\Gamma.$$

Finally, assume that the upright quarter is a loop with four or more upright quarters. Lemma 13.5 limits the possibilities to parameters (5, 0) or (5, 1). In the case of a loop (5, 1), there is no need to erase because $|V| \leq 3$ and by Lemma 13.5 the hexagonal standard region squanders at least

$$t_6 + 3a(p_v)\, pt$$

as required by the lemma. In the case of a loop (5, 0) in a pentagonal region, if $|V| = 1$ then there is no need to erase (again we appeal to Lemma 13.5). If $|V| = 2$, then the two vertices share a penalty of $4\xi_V + \xi_\Gamma$, with each receiving

$$2\xi_V + \xi_\Gamma/2 < 2\xi_V + \xi_\Gamma. \qquad \square$$

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Received November 11, 1998, *and in revised form September* 12, 2003, *and July* 25, 2005.
Online publication February 27, 2006.