Delaunay configurations and lipschitzian crowded sphere packings

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Abstract

This paper investigates the Delaunay configurations arising in a wide class of maximal sphere collections ruled by two parameters σ (spacing) and λ (Lipschitz). By means of lifting transforms, we show that the placement problem can be rephrased as the analysis of the space enclosed between two envelopes of half-cones. Lower bounds on plane angles are established for all $\sigma > \lambda\sqrt{2}$ and they hold in any dimension. Besides, we exhibit critical configurations approaching them.

Keywords. Angle–bounded Delaunay meshes, sphere packings, placements, Voronoi diagrams of spheres, merged cone envelopes.

Background

Research in sphere packings has been very active over the last decades. They occur in several fields of chemistry, physics and statistics [7, 11, 13, 16] ... Major results [1, 9] — including algorithms — have been obtained in the approximation of analytic functions through circle packings. However, application to mesh generation is quite recent: initiating the trend, Bern, Mitchell, and Ruppert [6] managed to triangulate polygons with acute angles by using linear–size packings.

Quality–guaranteed meshes of moderate size are mostly needed in finite–element methods: Miller, Talmor et al. [14, 15] lately introduced the interesting class of lipschitzian crowded packings. Although their concern was rather algorithmic (mesh corsening applied to numerical analysis), they established a lower bound of $1/(2-6\lambda)$ on Delaunay angle sines for $\sigma = 1$ and all $\lambda < 1/3$.

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In this paper, we present a general technique for excluding Delaunay configurations, thereby improving the angle bound for all $\sigma > \lambda\sqrt{2}$. Section 1 investigates the placement problem raised by the maximality assumption; it is answered constructively by means of lifting tranforms. Section 2 is dedicated to the study of angle bounds; we also examine critical configurations to estimate their tightness.

Basics

In the euclidian affine space $\mathbb{R}^{\mathrm{d}}$, $\overline{pq}$ denotes the distance between two points or the centers of two spheres p and q. The center and radius of any sphere s are respectively denoted by $\widehat{s}$ and $\mathrm{r}(s)$; for $\alpha \in \mathbb{R}^+$, αs means the sphere with center $\widehat{s}$ and radius $\alpha\mathrm{r}(s)$. Π being a collection of non–degenerate spheres, its *carrier* $\widehat{\Pi}$ is the set of its centers and $\alpha\Pi$ is defined as $\{\alpha s : s \in \Pi\}$.

We say that Π is *σ–spaced* and *λ–lipschitzian iff*:

$$\forall\,(p,q) \in \Pi^2,\ p \neq q:\ \ \mathrm{r}(p)+\mathrm{r}(q) \leq \sigma\,\overline{pq} \ \text{ and } \ |\mathrm{r}(p)-\mathrm{r}(q)| \leq \lambda\,\overline{pq} \quad (1)$$

Both parameters are assumed to be tight; hence $\lambda < \sigma$. In particular, Π is a *packing* if $\sigma < 1$; no sphere is included in another if $\lambda < 1$; no sphere contains a sphere center but its own if $\sigma - \lambda < 2$. If some sphere s may be added to Π without increasing either parameter, s is said to be *compatible* with Π; its center is then called a *placement.* Π is *crowded* over a domain Ω of $\mathbb{R}^{\mathrm{d}}$ *iff* no placement is possible in Ω.

1 Placements

1.1 Characterization

Lemma 1 — *ω is a placement for Π iff:*

$$\forall\,(p,q) \in \Pi^2, \quad \mathrm{r}(p)+\mathrm{r}(q) \leq \sigma\,\overline{p\omega} + \lambda\,\overline{q\omega}$$

Proof — Let ω be a candidate point and:

$$\rho^- = \max_{p\in\Pi}\left(\mathrm{r}(p) - \lambda\,\overline{p\omega}\right) \quad \text{and} \quad \rho^+ = \min_{q\in\Pi}\left\{\sigma\,\overline{q\omega} - \mathrm{r}(q),\ \mathrm{r}(q) + \lambda\,\overline{q\omega}\right\}$$

According to Inequations (1), the sphere s with center ω and radius $\rho > 0$ is compatible with Π *iff* $\rho^- \leq \rho \leq \rho^+$. The parameter ρ may be eliminated: ω is a placement *iff* $\rho^- \leq \rho^+$ and $\rho^+ > 0$. The four underlying inequalities are easy to check. ∎

Lemma 1 implies that *scaling preserves placements*; indeed, the packing Π/σ has Lipschitz factor λ/σ.

The *forbidden zone* of Π — complementary to the placement zone — may be viewed as the union of bounded loci O_{pq} warded by each $(p,q) \in \Pi^2$: $O_{pq} = \{\, \omega \in \mathbb{R}^{\mathrm{d}} : \sigma\, \overline{p\omega} + \lambda\, \overline{q\omega} < \mathrm{r}(p) + \mathrm{r}(q) \}$.

PROPERTY 1 — *O_{pq} is non–empty* iff $\lambda\, \overline{pq} < \mathrm{r}(p) + \mathrm{r}(q)$. *It is then an oval revolution body around line $(\widehat{p}, \widehat{q})$, and the only sphere center it contains is $\widehat{p}$.*

<u>Proof</u> — Two of the assertions are trivial:

$$\forall s \in \Pi \setminus \{p\},\ \sigma\, \overline{ps} + \lambda\, \overline{qs} \geq \mathrm{r}(p) + \mathrm{r}(s) + |\mathrm{r}(q) - \mathrm{r}(s)| \geq \mathrm{r}(p) + \mathrm{r}(q)$$

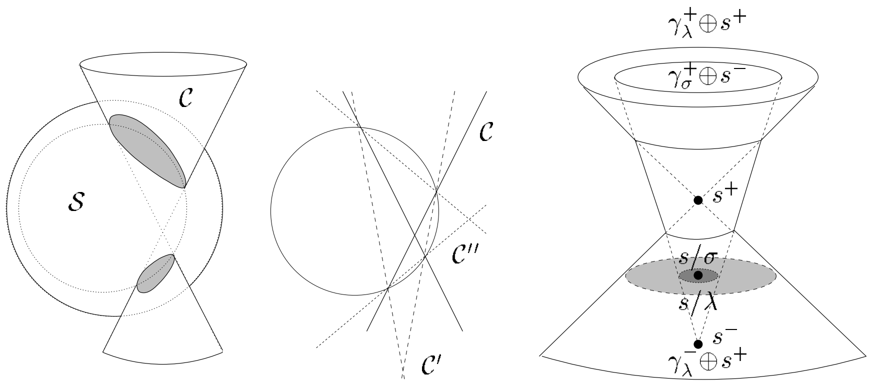
$$\widehat{p} \notin O_{pq} \ \Rightarrow\ \forall \omega \in \mathbb{R}^{\mathrm{d}},\ \mathrm{r}(p) + \mathrm{r}(q) \leq \lambda\, \overline{pq} \leq \lambda\, (\overline{p\omega} + \overline{q\omega}) \ \Rightarrow\ O_{pq} = \emptyset$$

In particular, O_{pq} is a ball if $\lambda = 0$, a solid ellipsoid as $\lambda \to \sigma$. Convexity follows from Lemma 2. The study of the quartic meridian curve — a so-called *Descartes oval* — shows that when $\lambda \neq 0$, the closest (resp. farthest) point to (resp. from) $\widehat{p}$ is the unique point achieving maximal (resp. minimal) local curvature. ∎

1.2 Lifting transforms

LEMMA 2 — *In $\mathbb{R}^3$, consider a sphere $\mathcal{S}$ and a revolution cone $\mathcal{C}$ whose apex lies strictly inside $\mathcal{S}$. Their intersection $\mathcal{I}$ consists of two simple closed curves; the projection parallel to the cone axis of either is a Descartes oval. Besides, there exist two other revolution cones $\mathcal{C}'$ and $\mathcal{C}''$ such that: $\mathcal{C} \cap \mathcal{C}' \cap \mathcal{C}'' \cap \mathcal{S} = \mathcal{I}$, all cones having parallel axes.*

This nice result from classical projective geometry implies that lifting transforms are the key to the placement problem. Completing the canonical basis of $\mathbb{R}^{\mathrm{d}}$ with the extra vector $\mathbf{u}$, let us map every sphere s of $\mathbb{R}^{\mathrm{d}}$ into two points in $\mathbb{R}^{\mathrm{d+1}}$: $s^- = \widehat{s} - \mathrm{r}(s)\, \mathbf{u}$ and $s^+ = \widehat{s} + \mathrm{r}(s)\, \mathbf{u}$. As s describes Π, two collections of points Π^- and Π^+ are obtained. The following result involves cone sweeps, so the Minkowski sum $\oplus$ provides handy notations. Given $t \in \mathbb{R}^+$, we denote by γ_t^- (resp. γ_t^+) the lower (resp. upper) sheet of the solid revolution cone of apex o (space origin), axis $\mathbf{u}$ and half-angle $\operatorname{arccot} t$.



(a) Cone/sphere intersection.

(b) Lifting transforms.

RESULT 1 — *Let $\mathcal{L}_\sigma = \gamma_\sigma^+ \oplus \Pi^-$ and $\mathcal{U}_\lambda = \gamma_\lambda^- \oplus \Pi^+$. Consider the zone where both half-spaces overlap and that enclosed in between: The projection of $\mathcal{L}_\sigma \cap \mathcal{U}_\lambda$ (resp. $(\mathcal{L}_\sigma \cup \mathcal{U}_\lambda)^{\complement}$) yields the forbidden (resp. placement) zone of Π. Besides, compatible balls are in bijection with the points enclosed between the half-spaces $\mathcal{L} = \mathcal{L}_\sigma \cup \mathcal{L}_\lambda$ and $\mathcal{U} = \mathcal{U}_\lambda \cup \gamma_0^-$, where $\mathcal{L}_\lambda = \gamma_\lambda^+ \oplus \Pi^+$.*

Proof — Following through the proof of Lemma 1, it is clear that the point of coordinates $[\omega, \rho^-]$ (resp. $[\omega, \rho^+]$) describes the boundary of $\mathcal{U}$ (resp. $\mathcal{L}$) as w sweeps $\mathbb{R}^d$. And two envelopes of head-to-foot half-cones suffice to determine placements. ∎

Recall that the arrangement induced by a collection of translated solid isotropic half-cones corresponds to the euclidian Voronoi diagrams of a set of spheres at all orders (that of order p is the labelled projection of level p — the locus of points belonging to exactly p half-cones). Therefore, in Result 1, the Voronoi diagrams of Π/σ, Π/λ and $-\Pi/\lambda$ are successively involved. The definition of the parameters of Π (Inequations (1)) is equivalent to the following properties: neither diagram has empty cells, i.e. vertices of Π^- (resp. Π^+) all lie on the boundary of $\mathcal{L}$ (resp. $\mathcal{U}$); and for all $p \neq q$, p^+ lies outside $\gamma_\sigma^+ \oplus q^-$.

2 Delaunay configurations

Property 2 — *The convex hull of a point subset Y of X defines a bounded face of the Delaunay complex of X* iff *there exists an empty open ball whose boundary contains exactly Y.*

This is the famous *empty–sphere criterion* [8]. Π is said to be *stable iff* its forbidden zone covers all Delaunay balls of $\widehat{\Pi}$ — we mean balls satisfying Property 2 for $\# Y > d$. In contrast, local configurations are excluded as follows: Consider a sphere collection Π_0 whose centers are cospherical on a ball b. We say that the configuration (Π_0, b) is (σ, λ)–*forbidden iff* no σ–spaced λ–lipschitzian sphere collection containing Π_0 and whose centers lie outside b is crowded over b.

2.1 Lower bounds on angles

2.1.1 Continuous approximation

The concept of forbidden configurations raises difficulties due to the σ–spacing condition (the "unknown" exterior spheres cannot be too close to each other). These may be overcome by making the problem "continuous": Consider the collection of *all* spheres centered outside b with maximal radii allowed by Π_0; it is given by the function ρ_M:

$$\rho_M : b^{\complement} \to]0, +\infty[, \quad p \mapsto \min_{s \in \Pi_0} (\mathrm{r}(s) + \lambda\, \overline{sp})$$

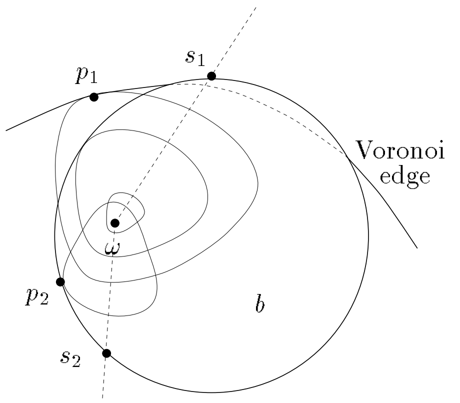
Lemma 3 — *If (Π_0, b) is (σ, λ)–forbidden, then:*

$$\forall\, \omega \in b,\ \exists\, (p, q) \in (b^{\complement})^2 : \sigma\, \overline{\omega p} - \rho_M(p) < \rho_M(q) - \lambda\, \overline{\omega q} \qquad (2)$$

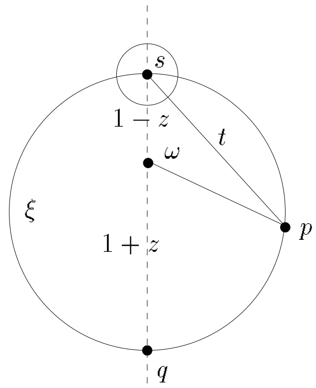
Proof — Assume that the inequality above does not hold for ω. According to Lemma 1, ω is a placement common to all sphere collections considered in the definition of forbidden configurations. ∎

The continuous approximation technique (CAT) then works as follows: Over $b^{\complement}$, find the infimum (resp. supremum) of the left (resp. right) member of Inequation (2). Then seek the optimal point ω^* minimizing the difference. An inequality involving σ, λ and metric characteristics of Π_0 will be obtained.

Function ρ_M involves a Voronoi diagram of spheres; the first step demands that extrema be computed over each of its cells (truncated



(c) Deep placements.



(d) One sphere case.

by b) — geometrically, this means solving contacts between Descartes ovals and hyperboloids (Voronoi facets) or the sphere bounding b: Unfortunately, the critical points p and q may not lie on the boundary of b. Excluding Delaunay faces (hence deriving lower bounds on solid angles directly) thus shapes up as a difficult challenge. Moreover, the following result justifies considering the case of one single sphere.

2.1.2 Threshold

Result 2 — *Let $\tau(\sigma, \lambda)$ be the optimal lower bound on angle sines obtained by considering one single sphere under the CAT. Then the CAT cannot provide a better bound than $\tau(\sigma, \lambda)/(1 - \lambda/\sigma)$ on angle sines for any $\lambda + \sigma < 2$.*

<u>Proof</u> — Our goal is to exhibit a σ–spaced λ-lipschitzian ball triad $\{p, q, s\}$ (unit circumball b) where $\mathrm{r}(p) = \mathrm{r}(s) + \lambda\, \overline{ps}$ and $\mathrm{r}(q) = \mathrm{r}(s) + \lambda\, \overline{qs}$ for arbitrarily small s. If such one exists, we claim that discarding p and q makes no difference for the CAT: In Lemma 3, p and q may indeed be blended with all points outside b (they are redundant with respect to s). Therefore the CAT cannot provide a better bound than $\min\{\overline{ps}, \overline{qs}\}/2$ on angle sines.

Take an iscoceles triangle whose basis $(\widehat{p}, \widehat{q})$ is as close to $\widehat{s}$ as possible: This is achieved for $\overline{sp} = 2\mathrm{r}(s)/(\sigma-\lambda)$, with $\mathrm{r}(p) = \mathrm{r}(q) = \frac{\sigma+\lambda}{\sigma-\lambda}\mathrm{r}(s)$.

It remains to check that: $\mathrm{r}(p)+\mathrm{r}(q)\leq\sigma\,\overline{pq}$ for arbitrarily small $\mathrm{r}(s)$, and as $(\sigma-\lambda)^2\,\overline{pq}=4\mathrm{r}(s)\,\sqrt{(\sigma-\lambda)^2-\mathrm{r}(s)^2}$, the condition simplifies to: $4\mathrm{r}(s)^2\leq(\sigma-\lambda)^2\left[4-(\sigma+\lambda)^2\right]$. ∎

2.1.3 Single sphere case

Take a single sphere s whose center lies on a unit sphere ξ (ball b). We expect a lower bound on $\mathrm{r}(s)$ depending on σ and λ by using the CAT. Lemma 3 implies that for all $\omega\in b$:

$$\inf_{p\in b\,\complement}(\sigma\,\overline{\omega p}-\lambda\,\overline{sp})+\lambda\inf_{q\in b\,\complement}(\overline{\omega q}-\overline{sq})<2\mathrm{r}(s) \tag{3}$$

By symmetry, we take ω on the diameter through $\widehat{s}$. Clearly, the second infimum $(-\overline{s\omega})$ is achieved for q lying diametrally opposite $\widehat{s}$. We claim that the critical point p lies on ξ: the Descartes ovals of equation $\sigma\,\overline{\omega p}-\lambda\,\overline{sp}=K$ indeed behave as collapsing contours as K diminishes; the point is that they vanish (at ω) *inside* b.

Parametrizing the position of p on ξ by $t=\overline{sp}$ and that of ω by its distance $z<1$ to the center of ξ, we have: $\overline{\omega p}^2=zt^2+(1-z)^2$. The function to minimize is: $f:[0,2]\to\mathbb{R}$, $t\mapsto\sigma\,\overline{\omega p}-\lambda\,\overline{sp}$. A quick study shows that if $z\leq\lambda^2/\sigma^2$, then f is decreasing. Otherwise its minimum $(1-z)\sqrt{\sigma^2-\lambda^2/z}$ is reached at $t_m=\lambda(1-z)/\sqrt{\sigma^2z^2-\lambda^2z}$, but this may be accepted only if $t_m<2$, i.e. if $z>z_0=\lambda/(2\sigma-\lambda)$.

But we always have $z_0>\lambda/\sigma$ and in brief, the sought minimum value is $f(2)=\sigma(1+z)-2\lambda$ if $z\leq z_0$ and $f(t_m)$ otherwise. Seeking the optimal deep placement ω, we consider both cases: In the first one, $2\mathrm{r}(s)$ is bounded below by $(\sigma+\lambda)z+\sigma-3\lambda$ by Inequation (3). Making z maximum, we set $z=z_0$, hence a bound for all $\sigma>2\lambda$: $\mathrm{r}(s)>2(\sigma-2\lambda)(\sigma-\lambda)/(2\sigma-\lambda)$.

In the second case, by Inequation (3), we obtain the minoration: $2\mathrm{r}(s)>(1-z)(\sqrt{\sigma^2-\lambda^2/z}-\lambda)$. Intending to maximize over $[z_0,1[$ that function of z — denoted by g —, we compute its derivative:
$2z\,g'(z)=2\lambda z+(\lambda^2(1+z)-2\sigma^2z^2)/\sqrt{\sigma^2z^2-\lambda^2z}$. By squaring, it yields a quartic polynomial whose coefficients are homogeneous in $\alpha=\lambda/\sigma$ — we are only interested in its greatest root z_α:

$$Q_\alpha(z)=4(1-\alpha^2)z^4-4\alpha^2(1-\alpha^2)z^3-\alpha^2(4-\alpha^2)z^2+2\alpha^4z+\alpha^4$$

Note that α^2 may be shortly expressed as a function of z_α; it is then easy to prove that $z_\alpha\geq z_0=\alpha^2$ and that z_α increases with α; ω moves even closer to $\widehat{s}$ and reaches it when $Q_\alpha(1) = 4(1-\alpha^2)(1-2\alpha^2) = 0$, i.e. when $\alpha = 1/\sqrt{2}$. Therefore:

RESULT 3 — *For all $\lambda/\sigma = \alpha < \sqrt{2}$, all inner angles in the Delaunay triangulation of stable σ–spaced, λ–lipschitzian sphere collections have a sine greater than $\tau(\sigma,\lambda) = (1-z)(\sqrt{1-\alpha^2/z}-\alpha)/2$, where z is the greatest root of the polynomial P_α.*

2.2 Critical stable configurations

In *wheels*, the carrier are the vertices of a regular polygon of side d (with unit circumradius) plus its center. We denote by R (resp. r) the radius of the central (resp. surrounding) ball(s). We set: $R-r=\lambda$ and $2r=\sigma d$ in order to σ and λ for parameters. We aim at maximizing r to make inner angles the smallest possible.

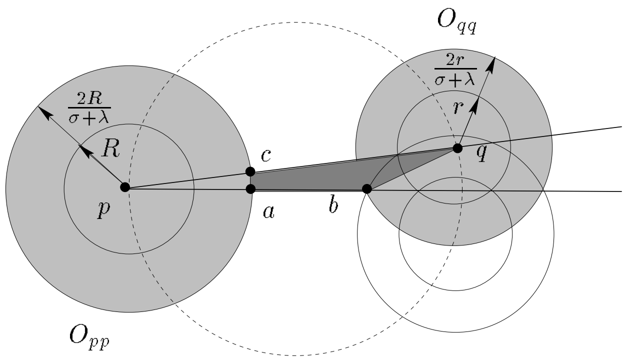


Figure 1: Wheel.

Refer to Figure 1. By symmetry, we examine the covering of one half-sector by the ovals $\{O_{pp}, O_{qq}, O_{pq}, O_{qp}\}$. We claim that $\{a,b\} \subset O_{qp}$ is a sufficient condition: Indeed, it implies $c \in O_{qp}$ as $\overline{pc} = \overline{pa}$ and $\overline{qc} < \overline{qa}$. And O_{qp} being convex, the convex hull of $\{q,a,b,c\}$ is then covered. Therefore, we apply Lemma 1 to a and b only, with $\overline{pa} = 2R/(\sigma+\lambda)$ and $\overline{qb} = 2r/(\sigma+\lambda)$:

$b \in O_{qp}$ *iff* $\lambda\,\overline{pb} < R - \frac{\sigma-\lambda}{\sigma+\lambda}r$. As $R = r+\lambda$, the condition becomes: $\overline{pb} < 1 + 2r/(\sigma+\lambda)$, which is always true! ($\overline{pb} < \overline{pq} = 1$). Thus, everything relies on the covering of the point a: $a \in O_{qp}$ *iff*:

$$\sigma\,\overline{qa} < r + \frac{\sigma-\lambda}{\sigma+\lambda}R \quad \text{with} \quad \sigma^2\,\overline{qa}^2 = r^2 + \left(\sqrt{\sigma - r^2} - \sigma\,\overline{pa}\right)^2$$

Hence $(3\sigma-\lambda)R^2-2(\sigma-\lambda)rR-(\sigma+\lambda)r^2+\sigma^2(\sigma+\lambda) \leq 4\sigma R\sqrt{\sigma^2-r^2}$. We eventually square again, with $R = r+\lambda$; we again obtain a quartic polynomial W. To put it in a homogeneous form, let $\alpha = \lambda/\sigma$ and $t = r/\sigma$. We may then conclude:

$$W_\alpha(t) = 16t^4 + 32\alpha t^3 - 16(1-2\alpha^2)t^2$$
$$-8\alpha(1-\alpha^2)(3-\alpha)t + (1+\alpha)(1-\alpha)^3(1+4\alpha-\alpha^2)$$

RESULT 4 — *For all $\lambda < \sigma$ there exist stable plane σ–spaced λ–lipschitzian sphere collections with Delaunay angles of sine equal to the smallest positive root of $W_{\sigma/\lambda}$.*

Conclusion

Next figure summerizes the different bounds obtained throughout Results 3 and 4. Combining Results 2 and 3, it is clear that the CAT cannot provide lower bounds on angles for $\sigma/\sqrt{2} \leq \lambda < \sigma$; closing this gap is a challenging open problem.

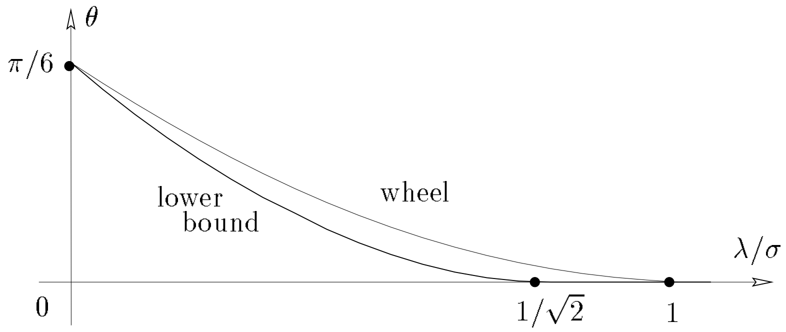


Figure 2: Angle bounds.

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