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Facet-Based Tetrahedralization Software

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#### Abstract

Soflware for computing Delaunay tetrahedralizations is described. The software is designed to be ased as part of a larger system and has a simple user interface. Numerically stable Householter transformations are used to implement orientation and insphere tests in floating-point arithmetic. A backward error analysis is done for the orientation test.


keywords: geometry software, Delanny tetrahedralization, Householder transformations, floatiug point arithmetic

## 1 Introduction

A Delaunay telrahedralization is a decomposition of the convex hull of a finite sfo of points in threwstimensional Fuclidean space into tetrahedra. It has an abundance of applications, including surface interpolation and finite-element mesh generation. We describe an implementation of a facet-based algorithm for computing Delaunay tetrahedralizations.

The software uses a simple algorithm that never deletes tetrahedra once they are discovered. Using a modification of Dwyer's[1] algorithm, the software starts with a briagular [ace of the convex liull and constructs a sequence of tetrahedra by repeatedly finding an apex for an exising Delanay facet. The apex calculation uses the orientation and insphere predicates.

The software is designed to be used as part of a larger system and has a well-defned user interface, where all communication is through the parameter list and no input or output is producect by the software. The tetrahedralization is represemed by two arrays containing vertex and adjacency information. Numprically stable Householder transformations are used in the floating-point implementations of the orientation and insphere tests and the giftwrapping primitive. The software was recently used by Frank Ray, a research scientist at McDonald Observatory, University of 'lexas at Austin, in the interpolation of thermal volumetric data in steel telescope prinary mirror structures[2]. C and Fortran code are available from the author.

A Delaunay letrahedralization can be computed directly in an incremmental fashion (Watson [3], Field[4], Cavendish et al, [5] and Rajan[6]). These methods begin with an initial tetratredratization of a few points and update the existing tetrahedralization as points are added. Dwyer|l] presents a linear expected time analysis of a facet-based technique for points uniformly distributed in a unit d-ball.

Cline and Renka[7] and Fortune[8] describe implementations of incromental twodimemsional Deftumy triangulation algorithons. Fortune[9] uses a sweep-line technique for computing Delammy triangulations. Renka's incrermental code[In] and Fortmen's sweppline code are available from nethb. CiPOMPAc'K by Barry Jop [1I] contans code for computing tetrahedralizations.

Many people have studied the problems of implementing geometric computations. Fortune and Van Wyk[12] develop efficient, exact arithmetic for geometric calculations. Edelsbrumner and Mücke[13] and Yap [14] perturb objects to avoid degeneracies.

Ottmann, Thient, and Ullrich[15], and Dobkin and Silver[16] use more than oue kind of arithmetic to achieve numerical stability for geometric computations. Hoffman, Hopcroft, and Karasick[17] maintain exact incidence information and approximate numerical information about objectis to achieve robust computations. Li and Milenkovic use rounded arithmetic to approximate curve arrangements[18] and convex hults.[19] Guibas, Salesin, and Stolif[20] use interval arithmetic and backward error analysis to produce the exact answer to a perturbed problem as well as a bound on the size of the perturbation. Fortune[21] analyzes floating point error for basic geometric calculations that are used in computing triangulations. Field[4] details a case study on the problems encountered in implementing Watson's algorithm for triangulations [3]. Hoffmann[22] compares several approaches and calls for more researeh on the topic of geometric computation.

In Section 2 the basic algorithm is presented; in Section 3 the implementation of floating point functions using Householder transformations is described; in Section 4 experimental results are reported.

## 2 Facet-Based Tetrahedralization

The three vertices of a lriangle uniquely determine a plane. The plane partitions $E^{33}$ into two open half spaces and the plane itself. The union of the plane and an open half space is a closed halr space. The triangle has two sides, one corresponding to each of the half spaces.

If a triangle is a facet of a tetrahedron, the tehrahedron is in exactly one of the closed half spaces defined by the facet, or on one side of the facet. The tetrahedron vertex that is not in the facet is called the apex of the facet.
pre: $P$ is set of $n$ points in $E^{3}$
post: $T$ is a Delautay tetrahedralization of $P$
less $(P, T)$
$T \leftharpoondown \theta_{i} \quad / / /$ known tetrahedra
$g$ ーinitial_facet; $\quad / /$ in boundary
$Q+g ; \quad / /$ pnol of facets
while $(Q \neq \emptyset)$ do
$f-\operatorname{front}(Q) ; \quad / /$ get an open facet
$a+$ getapex $(f) ; \quad / /$ find its apex
$t-\operatorname{conv}(f \cup\{a\}) ; \quad / /$ new tetrahedron
$T-T \cup\{t\} ;$
for $g$ a facet of $l$ do
if $(g \notin Q)$
then $Q-Q \cup\{g\} ; \quad / / \mathrm{g}$ is open
else $Q-Q-\{g\} ; \quad / / \mathrm{g}$ now closed
Figure 1: Facet-Based Delaunay 'Tetrahedralization

Lemma 1 provides a basis for the algorithm shown in Figure 1
Lemma 1 In a tctruhedralization of $P$, every facet of a tetrahedron is either a farel of exactly two tefrahedra, or in the boundary of the convex hull of $P$ and a facet of exactly one trimhedron.

As illustrated in Figure 2, the algorithm first finds a facet $g$ of a letrahedron $s$ in $T$ that lies in the boundary of the convex hull of $P$. All the points of $P$ are on one side of $g$. Then the apex $c$ of $g$ in $s$ is found
among the points of $P$. Let $\int$ be a facet of $s$ that contains $c$, let $b$ be the apex of $f$ in $s$, and let $A$, be the set of points of $P$ that are on the opposite side of $f$ from $b$. If $A$ is empty, $f$ is in the boundary and all of its tetrahedra have been found. Otherwise, there is another tetrahedron $t$ that contains $f$, and its apex a must be found. The facets of $t$ that contain $a$ will be explored, in turn, to see if they form part of the boundary or yield yet another tetrahedron. As the process continues, the construction may wrap back on itself so that tetrahedron $t$ has already been found and no construction is necessary. The algorithm terminates when no unexplored facets are left.


Figure 2: Basic Tetrahedron Construction
Since a Delaunay tetrahedralization induces a Delaunay triangulation on the facets of the convex hull, an initial facet can be obtained by computing a convex hull facet, and, if necessary, a Delaunay triangulation of the facet. The giftwrapping algorithm [23] provides a convenient way to compute a single convex hull facet.

Although every facet in a Delaunay tetrahedralization of $P$ has the property stated in Lemma 1, while the algorithm is exccuting, the information we have at hand is incomplete. Each facet falls into one of three categories:

- unknown: the facet belongs to no tetrahedron (facet y in Figure Za)
- open: the facet belongs to one known tetrahedron and no boundary information is known, or the facet belongs to no known tetrahedra and is known to be in the boundary (initial facet only) (facet. $f$ in Figure 2c, facet $g$ in Figure 2a)
- closed: the facet belongs to two known tetrahedra, or the facet belongs to one known tetrahedron and is known to be in the boundary (facets $f$ and $g$ in Figure 2d)

Open facets are kept in a queue, which is implemented as a hash table for faster searching.
Apex construction depends on the following properties of intersecting laalls.
Lemma 2 If two balls $B$ and $C$ interseat, their intersection is a disk $D$. The disk determines a plane and open half spaces. $H^{+}$and $H^{-}$. Let $B^{ \pm}=B \cap H^{ \pm}$and $\left(^{ \pm}=C^{\prime} \cap H^{ \pm}\right.$. Then exactly one of the assertions $B^{+} \subset C^{+}$and $C^{+} \subset B^{+}$is true, and the inclusion is reversed in $H^{-}$. That is, if $B^{+} \subset C^{+}$, then $\mathrm{C}^{-} \subset B^{-}$, and if $\mathrm{C}^{+} \subset B^{+}$, then $\mathrm{R}^{-} \subset \mathrm{C}^{-}$.

Lemma 3 Let $f$ be a traangle in $f^{3}, I^{+}$an open halfspace determuned by $f$, and let $\mathcal{L}$ be the line through the circumeenter of and normal to $f$. For point a in $H^{+}$, let $C_{a}^{\prime}$ be the ball defined by a and the vertaces of $f$ with center $c_{a}$ and radius. $r_{a}$ and let $\left(i_{a}^{+}=C_{a} \cap H^{+}\right.$. Inpose a one-dimensional coordinate systrm on $\mathcal{L}$ with 0 in the plane of $f$ and positive direction in $\mathrm{H}^{+}$, and let $L_{a}$ be the $\mathcal{L}$-coordinate of $\mathrm{C}_{a}$.

If $a$ and $b$ are pounts in $I^{+}$, then $L_{a}<l_{b}$ if and ouly if $C_{a}^{+} \subset C_{b}^{+}$
Proof: Let $\ell_{n}^{ \pm}\left(\ell_{b}^{ \pm}\right)$be the intersection of the boundary of $C_{a}^{\prime}\left(C_{b}\right)$, line $\mathcal{L}$, and halfspace $H^{ \pm}$. By Lemina 2 it suffices to show that $\ell_{a}^{+}$is closer than $\ell_{b}^{+}$to $f$, or that $\ell_{b}^{-}$is closer than $\ell_{a}^{-}$to $f$. The distance from $\ell_{a}^{ \pm}$ to $f$ is $r_{a} \pm \ell_{a}$, and the distance from $\ell_{b}^{ \pm}$to $f$ is $r_{b} \pm L_{b}$. If $r_{a}<r_{b}$, then $r_{a}+L_{a}<r_{b}+L_{b}$, so $\ell_{a}^{+}$is closer than $f_{b}^{+}$to $f$. If $r_{b}<r_{a}$, then $r_{b}-L_{b}<r_{a}-L_{a}$, so $\digamma_{b}^{-}$is closerer than $\rho_{a}^{-}$to $f$.

This result yields in a straightforward manner a characterization of the apex of a facet in a Delaunay tetrahedralization.

Theorem 1 Let $f$ be a facet in a Delaunay tetrahedralization, and let $P^{+}$be the subset of $P$ on one side of $f$. If $P^{+}$is emply, then $f$ is a boundary facet. Otherwise a point of $P^{+}$that generates the center of minimum $\mathcal{L}$-coordinate is the apex of facet $f$ in a Delaunay tetrahedralization.

Theorem 2 Algorithm tess shown in Figure 1 produces a Delaunay tetrahedralization of $P$ in $O\left(n^{2}\right)$ space and $O\left(n^{3}\right)$ time in the worst case.

Proof: By Theorem 1 each tetrahedron producd by algorithm tess is a Delaunay tetrahedron. These tetrahedra intersect in mutual faces and have circumballs, the interiors of which are free of points of $P$. If the convex hull of $P$ is not covered by these tetrahedra, by Lemma 1 there will be at least one facet interior to the convex hull of $P$ that belongs to exactly one tetraledron. This is impossible, since open facets remain in the facet pool and prevent termination of the algorithm, so the convex hull of $P$ is covered by tetrahedra and that $P$ is the set of vertices of tetrahedra.

Since no facet is added to the pool more than once, and a facet is removed in each iteration, the while loop, and therefore the algorithm, terminate.

Construction of the initial facet requires $O(n)$ time. Finding the apex of a single tetrahedron requires $O(n)$ time. The number of Delaunay tetrahedra in a tetrahedralization of $n$ points can be as great as $O\left(n^{2}\right)$ [24].

For many point sets the Delaunay tetrahedralization has size $O(n)$.
Corollary 1 If the size of the tetrahedralization is $O(n)$, algorithm tess requires $O(n)$ space and $O\left(n^{2}\right)$ time.
A Delaunay tetrahedralization is unique unless five or more points of $P$ lie on the circumball of a tetrahedron. The convex hull of the points on the circumball define a unique polytope, any tetrahedralization of which is a Delaunay tetrahedralization. It is possible for several points to generate the minimum $\mathcal{L}$ coordinate, and therefore lic on a common sphere. Any of the points can be used as the apex, since this is exactly the situation where the Delaunay tetrahedralization is not unique. However, our algorithm can cover the convex hull with multiple sets of tetrahedra. The two-dimensional example in Figure 3 illustrates the problem. In the two-dimensional case, facets are edges of triangles. Eventually $\triangle a b c, \Delta a c d, \Delta a b d$, and

open facets in the queue $Q=\{\overline{a b}, \overline{a d}\}$
$c$ is found as an apex for $\overline{a b} \quad Q=\{\overline{a d}, \overline{b c}, \overline{a c}\}$
$b$ is found as an apex for $\overline{a d} \quad Q=\{\overline{b c}, \overline{a c}, \overline{a b}, \overline{b d}\}$

Figure 3: Problem with Cospherical Points
$\Delta b c d$ will be added to the tetrahedralization. The convex hull of the cospherical points is covered with two sets of triangles, and facet $\overline{a b}$ is incorrectly added to the queue for a second time.

This problem can be avoided by enforcing some consistent method for choosing an apex. One method is illustrated in Figure 4. Let, $A$ be the set of points that generate the minimum $\mathcal{L}$-coordinate with respect to facet $f$, and let $B=A \cup\{$ vertices of $f\}$. Let, a be the point of minimum index in $P$ among the points of $B$. We arbitrarily choose the apex in that point $a$ is a vertex of every tetrahedron with vertices in $B$. If $a$ is

b

$$
\begin{array}{ll}
A=\{a, b, c, d\} & A=\{b, c, d, c\} \\
B=\{a, b, c, d, e, g\} & B=\{a, b, c, d, c, g\} \\
a \notin f \text { so choose } a & a \in \int \text { so choose } f
\end{array}
$$

Figure 4: Solution to Cospherical Points
in $A$, choose $a$ as the apex of $f$; if $a$ is a vertex of $f$, choose the point of minimum index that giftwraps the edge of $f$ that does not contain $a$.

Further investigation is needed to see if other selection criteria may be more desirable.

## 3 Using Householder Transformations

Geometric problems are often poorly conditioned in the sense that a small change in problem parameters may result in a large difference in the answer [25]. As an example, consider the computation which, given a line and a point, returns the value true if the point is on the line and false otherwise. A slight perturbation of the coordinates of the point or the coefficients of the equation of the line may change the result from false to true.

Floating point computations in our algorithm are confined to a variant of the orientation test, in which we test if two points lie on opposite sides of a plane (opp test); a rariant of the insplere test. namely the $\mathcal{L}$ coordinate calculation for determining an apex of a facet; and the giftwrapping primitive. Here we present an implementation of the opp test and apex computation using numerically stable Householder transformations (Stewart [26], Golub and Van Loan [27]), and hased on a development hy Alan C'line [28]. The giftwrapping primitive is similar to the apex computation.

Householder transformations, also known as elementary reflechors or elementary Hermitian matrices, have the form $Q=I-2 u u^{T}$, where $I$ is the identity matrix and $u^{T} u=1$, and are numerically stable, orthogonal $\left(Q^{T} Q=I\right)$, symmetric, and isometric (for any vector $\left.y,\|y\|=\|Q y\|\right)$ in the Euclidean norm. Geonetrically. when $Q$ is applied to a vector $v, v$ is reflected in the plane normal to $u$.

### 3.1 Opp Test

Given points $z_{1}$ and $z_{2}$, and a facet with non-collinear vertices $p_{1}, p_{2}$, and $p_{3}$, the opp test returns the value true if $z_{1}$ and $z_{2}$ are on the same side of the plane defined by the lacet and false otherwise. lect $P$ be the matrix $\left[p_{2}-p_{1} p_{3}-p_{1}\right]$, and compute the Householler $Q R$ factorization [27], [26] to obtain $P=Q_{1} Q_{2} R$, where $Q_{1}, Q_{2}$ are Householder transformations and $R$ is upper triangular. If $v=Q_{1} Q_{2} e_{3}$, where $e_{3}=(0,0,1)^{T}$, then $v$ has unit length, since $Q_{1}$ and $Q_{2}$ are isometric. In addition,

$$
P^{T_{v}}=R^{T} Q_{2} Q_{1} v=R^{T} c_{3}=0
$$

since the third row of $R$ is 0 . That is, $v$ is a unit normal to the facet. Therefore, points $z_{1}$ and $z_{2}$ are on the same side of the plane defined by $p_{1}, p_{2}$, and $p_{3}$ if and only if the signs of $\left(z_{1}-p_{1}\right)^{T} v$ and $\left(z_{2}-p_{1}\right)^{T} p$ are the same.

For backward error analysis of the opp test, we want to show that the computed answer is the exact answer to a slightly perturbed problem. The opp test requires the following computations: compute $Q_{1}$; compute $Q_{2} ; v ゅ Q_{1} Q_{2} e_{3}$; compare $\left(z_{1}-p_{1}\right)^{T} v$ and $\left(z_{2}-p_{1}\right)^{T} v$. Following Fortune, [21] we use approximate arithmetic, or floating-point arithmetic without underflow or overflow, with error bound $\epsilon_{0}$ on a single arithmetic operation. The comparison can be done exactly, so we need only analyze a computation of the Гorm $(z-p)^{T} Q_{1} Q_{2} \mathrm{e}_{3}$.

We first examine separately the errors incurred by approximate arithmetic in computing dot products, vector difference, Householder transformations, and vector multiplication by a product of Householder transformations. Where there is a choice, we amortize the error uniformly over the appropriate values.

Consider the dot product computation $\sum_{i=1}^{n} a_{i} b_{i}$. Let $s$ be the result computed in approximate arithmetic. Using standard techniques it can be shown that

$$
s=\sum_{i=1}^{n} a_{i}\left(1+\theta_{i}\right) b_{i}\left(1+\theta_{i}\right)
$$

where $\left|\theta_{i}\right| \leq(n-i+3) \epsilon_{0} / 2$ for $i=1, \ldots, n$. In this context, $n=3$, so $\left|0_{i}\right| \leq 5 \epsilon_{0} / 2$ for $i=1, \ldots, 3$.
Let $d$ be the difference between two vectors, $a-b$, computed in approximate arithmetic. From the bound on approximate arithmetic $d=a\left(1+u_{a}\right)-b\left(1+u_{b}\right)$, where the components of error vectors $u_{a}$ and $u_{b}$ have absolute value less than $\epsilon_{0}$.

Suppose $\hat{Q}$ is a computed Householder transformation of order three. Accorcling to Golub and Van Loan,[27], if $m$ is the computed result of multiplying 3 -vector $v$ by $\dot{Q}$. then $m=Q(v+e)$, where $\|e\| \leq$ $9 c c_{0}\|v\|$, and $c$ is a constant of order unity. Applying this to the computed value $t$ of $Q_{1} Q_{2} x$, wo have $t=$ $Q_{1}\left(Q_{2}\left(x+f_{2}\right)+f_{1}\right)$, where $\left\|f_{2}\right\| \leq 9 c \epsilon_{0}\|x\|$ and $\left\|f_{1}\right\| \leq 9 c c_{0}\left\|Q_{2}\left(x+f_{2}\right)\right\| \leq 9 c \epsilon_{0}\left\|x+f_{2}\right\| \leq 9 c \epsilon_{0}\|x\|\left(1+9 c c_{0}\right)$, since $Q_{2}$ is isometric. Finally, $t=Q_{1}\left(Q_{2}\left(x+f_{2}\right)+f_{1}\right)=Q_{1} Q_{2}(x+h)$, where $h=f_{2}+Q_{2}^{T} f_{1}$, and $\|h\| \leq 9 c \epsilon_{0}\|x\|\left(2+9 c \epsilon_{0}\right) \leq 27 c \epsilon_{0}\|x\|$.

Let $r$ be the computed result of $(z-p)^{T} Q e_{3}$, where $Q=Q_{1} Q_{2}$. Using the above results, $r=\sum_{i=1}^{3}\left[\left(z_{i}(1+\right.\right.$ $\left.\left.\left.u_{z}\right)-p_{i}\left(1+u_{p}\right)\right)(1+\theta)\right] \cdot\left[\left(Q\left(e_{3}+f\right)\right)_{i}(1+\theta)\right]$, where $\left|u_{z}\right| \leq \epsilon_{0},\left|u_{p}\right| \leq \epsilon_{0},|\theta| \leq 5 \epsilon_{0} / 2$, and $||f|| \leq 27 c \epsilon_{0}| | e_{3}| |=$ $27 c \epsilon_{0}$.

Now $z_{i}\left(1+u_{z}\right)(1+\theta)=z_{i}(1+\delta)$, and $p_{i}\left(1+u_{p}\right)(1+\theta)=p_{i}(1+\delta)$, where $|\delta| \leq 4 \varepsilon_{0}$.
Furthermore, $\left(Q\left(c_{3}+f\right)_{i}(1+\theta)=\left(Q e_{3}\right) i+\left(Q e_{3}\right)_{i} \theta+(Q f)_{i}+(Q f)_{i} \theta=\left(Q e_{3}\right)_{i}+d_{1}\right.$, where $\|d\| \leq$ $\epsilon_{0}+27 \epsilon_{0}+27 \epsilon_{0}^{2} \leq 29 \epsilon_{0}$. Reassembling vectors from components, $\left(Q\left(e_{3}+f\right)\right)(1+\theta)=Q\left(e_{3}+f\right)+d=$ $Q\left(e_{3}+f\right)+Q g=Q\left(\epsilon_{3}+h\right)$, where $\|h\|=\|J\|+\|g\| \leq 27 c \varepsilon_{0}+\|d\| \leq 56 c \epsilon_{0}$.

Finally,

$$
r=\sum_{i=1}^{3}\left[z_{i}(1+\delta)-p_{i}(1+\delta)\right] \cdot\left[\left(Q\left(c_{3}+h\right)\right)_{i}\right]
$$

where $|\delta| \leq 4 \epsilon_{0}$ and $\|h\| \leq 56 c{ }^{\circ}$. 'That is, the computed value of the opp test is the exact value of a slightly perturbed problem.

## $3.2 \mathcal{L}$-coordinates

As discussed previously, the aprex of a facet is the point that generates a center of minimum $\mathcal{L}$-coordinate among all the points on one side of the facet, say in $H^{+}$. If we fix a facet with theee non-collinear vertices $p_{1}, p_{2}$, and $p_{3}$, then we can define a function $L$ that associates a point $p$ in $p^{+}$with the $\mathcal{L}$-coordinate of the center of the circumball defined by $p, p_{1}, p_{2}$, and $p_{3}$. The function $L$, can also be implemented with Honseholder transformations. We compute $a$ a unit, normal to the facet, $c$, the circumcenter of the facet, and finally the $\mathcal{L}$-coordinate of the center of the ball. In practice $v$ and $c$ are computed once for each facet. Factor $P=\left[\begin{array}{ll}p_{2}-p_{1} & p_{3}-p_{1}\end{array}\right]$, so $P=Q_{1} Q_{2} R$, where $Q_{1}, Q_{2}$ are Householder transformations and $R$ is upper triangular, and let $Q=Q_{1} Q_{2}$. As in the opp test, the unit normal is $Q_{1} Q_{2} e_{3}=Q \epsilon_{3}$. Since $c$ is in the plane of the facel, $c-p_{1}$ can be written as $Q y$, where the third component of $y$ is 0 . Then

$$
\left\|c-p_{1}\right\|=\left\|Q_{y}\right\|=\|y\|
$$

since $Q$ is isometric. For $j=1,2$, the $j$-th column of $P$ can be written as $p_{j+1}-p_{1}=P e_{j}=Q R e_{j}=Q r_{j}$, where $r_{j}$ is the $j$-th column of $R$. Therefore,

$$
\begin{equation*}
\left\|c-p_{j+1}\right\|=\left\|\left(c-p_{1}\right)-\left(p_{j+1}-p_{1}\right)\right\|=\left\|Q y-Q r_{j}\right\|=\left\|y-r_{j}\right\| \tag{1}
\end{equation*}
$$

Since $c$ is the circumcenter of the facet, it is equidistant from the vertices, and, for $j=1,2,\|y\|=\left\|y-r_{j}\right\|$. Since $R$ is upper triangular, when $j=1$,

$$
y_{1}^{2}+y_{2}^{2}=\left(y_{1}-r_{11}\right)^{2}+y_{2}^{2}
$$

yielding

$$
y_{1}=r_{11} / 2
$$

and, when $j=2$,

$$
y_{1}^{2}+y_{2}^{2}=\left(y_{1}-r_{12}\right)^{2}+\left(y_{2}-r_{22}\right)^{2}
$$

yielding

$$
y_{2}=\left(r_{22}+\left(r_{12} / r_{22}\right)\left(r_{12}-2 y_{1}\right)\right) / 2
$$

Now we are able to compute $Q y$ to obtain $c$, the center of the facet
The center $s$ of the ball can be written as $c+\mathcal{L} v$, where $\mathcal{L}$ is the $\mathcal{L}$-coordinate of $s$. Since $s$ is equidistant from $p_{1}$ and $p$,

$$
\begin{aligned}
\left\|s-p_{1}\right\| & =\left\|s-p^{\prime}\right\| \\
\left\|(c+\mathcal{L} v)-p_{1}\right\| & =\|(c+\mathcal{L} v)-p\| \\
\left\|\left(r-p_{1}\right)+\mathcal{L} v\right\| & =\left\|\left(c-p_{1}\right)-\left(p-p_{1}\right)+\mathcal{L} v\right\|
\end{aligned}
$$

Writing $Q^{T}\left(p-p_{1}\right)$ as $r$, we have $Q^{T}\left(p-p_{1}\right)=r=Q^{T} Q r$, and $\left(p-p_{1}\right)=Q r$. Recalling that $\left(r-p_{1}\right)=Q y$ and $v=Q e_{3}$, we get.

$$
\left\|Q y+\mathcal{L Q} Q e_{3}\right\|=\left\|Q y+\mathcal{L} Q e_{3}-Q r\right\|
$$

and

$$
\left\|Q\left(y+\mathcal{L} e_{3}\right)\right\|=\left\|Q\left(y+\mathcal{L} e_{3}+r\right)\right\|
$$

Since $Q$ is orthogonal,

$$
\left\|y+\mathcal{L} e_{3}\right\|=\left\|y+\mathcal{L} e_{3}+r\right\|
$$

Sguaring both sides we get

$$
\left(y+\mathcal{L} \ell_{3}\right)^{T}\left(y+\mathcal{L} f_{3}\right)=\left(y+\mathcal{L} r_{3}-r\right)^{P}\left(y+\mathcal{L} r_{3}-r\right) .
$$

which reduces to

$$
0=r^{T} r-2 r^{T} y-2 \mathcal{L} r^{T}+3
$$

Hence

$$
\mathcal{L}=\frac{\|r\|^{2}-2 y^{T} r}{2_{3}^{T} r}
$$

This can be simplified using:

$$
\begin{gathered}
\|r\|^{2}=\left\|p-p_{1}\right\|^{2}=\left(p-p_{1}\right)^{T}\left(p-p_{1}\right) \\
e_{3}^{T}=e_{3}^{T} Q^{T}\left(p-p_{1}\right)=\left(Q e_{3}\right)^{T}\left(p-p_{1}\right)=v^{T}\left(p-p_{1}\right)
\end{gathered}
$$

and

$$
y^{I} r=\|^{T} Q^{T}\left(p-p_{1}\right)=(Q y)^{T}\left(p-p_{1}\right)=\left(c-p_{1}\right)^{T}\left(p-p_{1}\right)
$$

to the final form

$$
\mathcal{L}=\frac{\left(p-p_{1}\right)^{T}\left(p-p_{1}\right)-2\left(c-p_{1}\right)^{T}\left(p-p_{1}\right)}{r^{\prime}\left(p-p_{1}\right)}
$$

## 4 Experimental Results

The insphere test was implemented with and without Basic Linear Algebra Subroutines (BLAS),[29] which abstract vector operations. The timings in Table 4 for the insphere lest were done on one node of an nCUBE model 2 E computer, which has a BLAS library available. The numbers represent average cost per function evaluation, amortizing the one-time setup over all trials.

| Householder <br> no | Householder <br> library <br> blas | Householder <br> fortran <br> blas |  |
| ---: | ---: | ---: | ---: |
| trials |  |  |  |
| 10000 | $0.2517753 \mathrm{E}-04$ | $0.4506951 \mathrm{E}-04$ | $0.7514621 \mathrm{E}-04$ |
| 20000 | $0.2530957 \mathrm{E}-04$ | $0.4506079 \mathrm{E}-04$ | $0.7512725 \mathrm{E}-04$ |
| 30000 | $0.2342186 \mathrm{E}-04$ | $0.4505925 \mathrm{E}-04$ | $0.7512100 \mathrm{E}-04$ |
| 40000 | $0.2423604 \mathrm{E}-04$ | $0.4506010 \mathrm{E}-04$ | $0.7511742 \mathrm{E}-04$ |
| 50000 | $0.2363036 \mathrm{E}-04$ | $0.4505702 \mathrm{E}-04$ | $0.7511496 \mathrm{E}-04$ |
| 60000 | $0.2439852 \mathrm{~F}-04$ | $0.4505553 \mathrm{E}-04$ | $0.7511338 \mathrm{E}-04$ |
| 70000 | $0.2416601 \mathrm{E}-04$ | $0.4505539 \mathrm{E}-04$ | $0.751234 \mathrm{E}-04$ |
| 80000 | $0.2408908 \mathrm{E}-04$ | $0.4505610 \mathrm{E}-04$ | $0.751202 \mathrm{E}-04$ |
| 90000 | $0.2411615 \mathrm{E}-04$ | $0.4505655 \mathrm{E}-04$ | $0.751133 \mathrm{E}-04$ |
| 100000 | $0.2421591 \mathrm{E}-04$ | $0.4505658 \mathrm{E}-04$ | $0.7511085 \mathrm{E}-04$ |

BLAS Timings

Table 1 contains runtime data on one node of the nCUBE 2E for the insphere test implemented with Householder transformations without BLAS and with determinants. The numbers again represent average cost per function evaluation, amortizing the one-time setup over all trials. Set-up for the Houselolder version includes computing the transformations; for the detcrmininants, the one-time cast is for computing the minors. The runtimes are ahout the same over a range of trial sizes.

To empirically test accuracy, we set up an insphere problem with coordinates less than two in ahsolute value with the origin on the splere, then let the test point approach the origin. Tests were run with 32 -bit arithmetic. The Householder version returned a result of zero for points within $10^{-7}$ of the origin, which is expected, since it uses differences between points: if point $p 1$ has coordinates around size one, and $p^{2}$ is within $10^{-7}$ of origin $p^{3}$, then $p 2-p 1$ and $p 3-p 1$ will have the same value in 32 -bit arithmetic. The determinants performed better than the Householder transformations in this case: giving correct signs for points within $10^{-14}$ of the origin.

As Fortune[21] observed, points that are close together but far from the origin pose mumerical difficulties. We constructed a serquence of insphere problems by starting with a set of point coordinates less than two in absolute value and trauslating the same coordinate of each point by increasing powers of 10 . The problems are solved using Houscholder transformations with and without BLAS and determinants using an Alpha running VMS with default compiler settings.

There is no difference in accuracy in these tests between the versions of the Householder implementation in 32 -bit arithmetic. The Houscholder versions fail at $10^{8}$ with a zero divide, which is the point at which the points become indistinguishatbe in this floating-point system. The determinant version fails at $10^{4}$ with an incorrect result.

The test was also run in 64-bit arithmetic with no BLAS. The Householder version has a zero divide at. $10^{16}$, while determinants fail at $10^{6}$ with an incorrect answer.

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| trials | Houscholder <br> no blas | Determinants |
| ---: | ---: | ---: |
| 100 | $0.2443675 \mathrm{E}-04$ | $0.2391187 \mathrm{E}-04$ |
| 200 | $0.2612430 \mathrm{E}-04$ | $0.2939204 \mathrm{~F}-04$ |
| 300 | $0.2310050 \mathrm{E}-04$ | $0.2755631 \mathrm{E}-04$ |
| 400 | $0.2431148 \mathrm{E}-04$ | $0.2691151 \mathrm{E}-04$ |
| 500 | $0.2335035 \mathrm{E}-04$ | $0.2684309 \mathrm{~F}-04$ |
| 600 | $0.2452692 \mathrm{E}-04$ | $0.2694426 \mathrm{E}-04$ |
| 700 | $0.2419856 \mathrm{~F}-04$ | $0.2724844 \mathrm{E}-04$ |
| 800 | $0.2406637 \mathrm{E}-04$ | $0.2639701 \mathrm{E}-04$ |
| 900 | $0.2413915 \mathrm{E}-04$ | $0.2696446 \mathrm{E}-04$ |
| 1000 | $0.2430852 \mathrm{E}-04$ | $0.2656197 \mathrm{E}-04$ |
| 10000 | $0.2547753 \mathrm{E}-04$ | $0.2705126 \mathrm{E}-04$ |
| 20000 | $0.2530957 \mathrm{E}-04$ | $0.2686962 \mathrm{~F}-04$ |
| 30000 | $0.2342186 \mathrm{E}-04$ | $0.2706156 \mathrm{E}-04$ |
| 40000 | $0.2423604 \mathrm{E}-04$ | $0.2579072 \mathrm{E}-04$ |
| 50000 | $0.2363036 \mathrm{~L}-04$ | $0.2643391 \mathrm{E}-04$ |
| 60000 | $0.2439852 \mathrm{E}-04$ | $0.2699300 \mathrm{E}-04$ |
| 70000 | $0.2416601 \mathrm{E}-04$ | $0.2661089 \mathrm{~F}-04$ |
| 80000 | $0.2408908 \mathrm{~F}-04$ | $0.2642198 \mathrm{E}-04$ |
| 900000 | $0.2411615 \mathrm{E}-04$ | $0.2636195 \mathrm{E}-04$ |
| 100000 | $0.2421591 \mathrm{E}-04$ | $0.263918: 3 \mathrm{E}-124$ |

Insphere T'innings on nCUBE

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