An Algorithm for Computing the Shortest Path of Three Spheres

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***Abstract*—Computing the Euclidean shortest path among a plural number of spherical balls is an interesting problem in 3D computer graphics. Finding the Euclidean shortest path of three spheres is fundamental to the more general *n*-sphere problem. In this paper, we develop an exact algorithm for computing the shortest path of three spheres in 3D space. The problem is firstly reduced to a corresponding problem of computing the shortest path of three coplanar circles, and turns out to a two points and one circle path planning problem. After applying the general root formula of the shortest path of two points and one circle together with the method of axis rotation, the algorithm is build. Empirical results accompany a brute force method for comparison have shown the correctness and effectiveness of the proposed algorithm. This result can be applied in 3D computer graphics, computer-aided design and the molecular geometry.**

***Keywords*—distance among spheres, path planning of spheres, computational geometry, molecular geometry**

I. INTRODUCTION

Computing the Euclidean shortest path of spherical balls is an interesting problem in 3D computer graphics [1,2]. The problem of finding the shortest path of three spheres is fundamental to the more general *n*-sphere problem. In this paper, we consider the problem of finding the shortest path of three spheres in 3D space. The problem can be defined as: given three mutually exclusive spheres in 3D space, find the shortest Euclidean path which linearly traverses from one point on the surface of the first sphere to one point on the surface of the second sphere and then continues to a point on the surface of the third sphere to complete the path. The path in this fashion is an open route, i.e., the end point need not coincide with the start point. The length of the path is the sum of the two links connecting the three spheres. Let such problem be denoted by Ψ_3 where the subscript "3" represents the number of spheres.

Many researches regard to computing the shortest path of 3D sphere are discussing the path between points on a spherical surface wherein the arc of the great circle passes through the two points is the shortest path between such two points [3-5]. Molecular geometry [6,7] is 3D arrangement of the atoms that constitute a molecule, inferred from the spectroscopic studies of the compound. The position of each atom is determined by the nature of the chemical bonds by which it is connected to its neighboring atoms. The molecular geometry can be described by the positions of these atoms in space, evoking bond lengths of two joined atoms, bond angles of three connected atoms, and torsion angles of three consecutive bonds. This paper provides an effective way in computing the shortest path of three spheres what if the three molecules can be embraced by three spherical balls.

To our knowledge, there is no previous work in providing an effective method computing the shortest path of three spheres in 3D space. Chou [8] had resolved the general root formula computing the shortest path of three circles in 2D plane. This paper is to evolve the contribution of Chou's [8] to 3D space.

The rest of this paper is organized as follows. Section 2 shows the problem of finding the shortest path of three spheres can be reduced to a corresponding problem of finding the shortest path of three coplanar circles. After resolved the three circles problem in 2D plane, by using coordinate rotations, the resolved points on the three circles can be restored to their original coordinates on the surface of the 3D spheres. Section 3 introduces the general root formula of the three circles problem in our previous work. Section 4 generalizes the algorithm which comprises the steps of transforming the three spheres problem to a three circles problem, resolving the three circles problem in 2D plane, and then restoring the results to their original spherical surfaces in 3D space. An example accompanies in Section 5 together with a brute force method which can identify the correctness and effectiveness of the proposed algorithm. Section 6 concludes the paper and points out the future work.

II. PROBLEM TRANSFORMATION

Assume the traversal order of three spheres, say, S_A, S_B and S_C be represented by $S_A - S_B - S_C$, obviously which is equivalent to that of $S_C - S_B - S_A$. Hence, there are three different combinations about the traversal order. Without loss of generality, in this paper, we choose the three combinations $S_A - S_B - S_C$, $S_B - S_A - S_C$ and $S_A - S_C - S_B$ for illustration. The Ψ_3 problem in 3D space can be mapped to a corresponding problem of finding the shortest path of three coplanar circles in 2D plane by the following lemma.

Lemma 1. *The Ψ_3 problem can be degenerated to the problem of finding the shortest path of three coplanar circles where the three centers of the three spheres constructs the co-plane.*

Proof. Since there exits one and only one plane which extends through the three centers of the three spheres, any point on the surface of the sphere out of the great circle on such co-plane can be projected to the inner part of the great circle, for illustration see Fig. 1 where $\overline{A^*A^{**}}$ is perpendicular to the face of the great circle C_A of sphere S_A. Similarly, $\overline{P^*P^{**}} \perp C_C$ and $\overline{B^*B^{**}} \perp C_B$. For any point on the surface of the sphere, say A^{**}, P^{**} and B^{**}, there exists at least one point, say A, P and B on the circumferences of great circles C_A, C_C and C_B respectively, such that $\left|\overline{A^*P^*}\right| < \left|\overline{A^{**}P^{**}}\right|$ and $\left|\overline{B^*P^*}\right| < \left|\overline{B^{**}P^{**}}\right|$. We have

$$\left|\overline{AP}\right| + \left|\overline{BP}\right| < \left|\overline{A^*P^*}\right| + \left|\overline{B^*P^*}\right| < \left|\overline{A^{**}P^{**}}\right| + \left|\overline{B^{**}P^{**}}\right|.$$

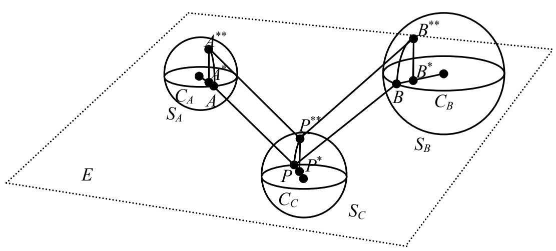

Figure 1. Three spheres and the co-plane.

For any point on the surface of the three spheres out of the circumferences of the three great circles constructs one path, we can find at least one path where the three points locate on the circumferences of the three great circles resulting in a shorter path. □

The Ψ_3 problem is now reduced to the problem of finding the shortest path of three coplanar great circles of the three spheres. After resolving the shortest path of the three circles problem in 2D plane, by using coordinates rotations, the resolved three contact points on the three circles in 2D coordinates can be restored to their original 3D coordinates accordingly. The steps of such coordinates rotations and restorations can be described as follows. When the co-plane E is obtained, we can rotate the axes to make xy-plane coincided with co-plane E. This generates a new coordinates system, say, $x''y''z''$-system with $z''=0$ on the co-plane E, where there exists linear transformation from the original xyz-system to the generated $x''y''z''$-system. Hence, if we are able to resolve the optimal contact point P'' in the new generated coordinates system, we can restore the coordinates of P'' back to its original coordinates of P by means of matrix inverse transformations [9].

We use orthogonal axes in this paper, the rotation about z-axis is positive if we perpendicularly see xy-plane from the positive direction of z-axis and the rotation is counterclockwise (CCW). On the contrary, the angle is negative if the rotation is clockwise (CW). If we want to make xy-plane completely coincided with plane E, we need to know two angles in advance, the included angle φ of the two planes, and the included angle ϕ of x-axis with respect to the line ζ which is the intersection of plane E and xy-plane see Fig. 2 for illustration.

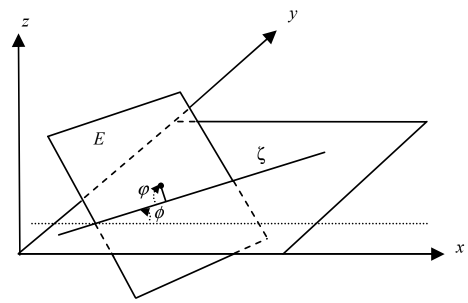

Figure 2. Two angles and the co-plane.

Let point P be in the original coordinates system, P' is its mapping in the rotated coordinates system for ϕ angle about z-axis, and R_z be a 3×3 transition matrix which transforms P to P', i.e., $R_z : P(x,y,z) \mapsto P'(x',y',z')$. This mapping can be represented by

$$P' = R_z \bullet P.$$

That is,

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

If we want to restore point P' back to the original coordinates system, it is obviously we use the inverse matrix of R_z which is denoted by R_z^{-1}. The next theorem shows the transition matrix from one orthonormal basis to another having a special property that makes its inverse easy to obtain [9].

Theorem 1. *If R is the transition matrix from one orthonomal basis to another orthonomal basis for an inner product space, then $R^{-1} = R^t$.*

According to theorem 1, we can easily obtain the inverse matrix of R_z by its transpose, i.e.,

$$R_z^{-1} = R^t = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

We get

$$P = R_z^{-1} \bullet P' \quad \Rightarrow \quad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}.$$

Similarly, with the same technology, rotating x'-axis about φ degree makes xy-plane completely stuck on plane E, we can use the mapping

$$P'' = R_x \bullet P' \quad \Rightarrow \quad \begin{bmatrix} x'' \\ y'' \\ z'' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{bmatrix} \bullet \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}.$$

And then we can restore P'' to its previous coordinates system by using the following mapping

$$P' = R_x^{-1} \bullet P'' \quad \Rightarrow \quad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{bmatrix} \bullet \begin{bmatrix} x'' \\ y'' \\ z'' \end{bmatrix}.$$

Combining the two steps of rotating about z-axis and x'-axis, which can be written by

$$P'' = R_x \bullet P' = R_x \bullet R_z \bullet P.$$

So that

$$P'' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & -\sin\varphi \\ 0 & \sin\varphi & \cos\varphi \end{bmatrix} \bullet \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet P. \quad (1)$$

While the optimal contact point P'' is obtained in the $x''y''z''$-system, we can directly restore it back to the original xyz-system by

$$P = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{bmatrix} \bullet P''. \quad (2)$$

Now that all the steps of rotations about the axes are clear. We can concentrate on solving the optimal contact points in 2D plane. After the optimal contact point P'' is obtained in the $x''y''z''$-system, we have evident steps restoring its coordinates back to the original P in the xyz-system.

III. THE THREE CIRCLES PROBLEM

After the Ψ_3 problem is reduced to the problem of finding the shortest path of three coplanar great circles of the three spheres. This section depicts the three circles problem in 2D and the general root formula in our previous work [8]. The three circles problem in 2D plane is defined as follows. Given three disjoint circles in 2D plane, find the path that traverses all three circles in a predefined sequence for which the sum of the two interconnecting links is a minimum. In that paper, this three circles traversal path problem can be further reduced to a corresponding problem of computing the traversal path of two points and one circle, see Fig. 4 for illustration. We use Q_1^2 to represent the problem for computing the shortest path of two points and one circle where the superscript "2" represents the two points whereas the subscript "1" indicates the one circle.

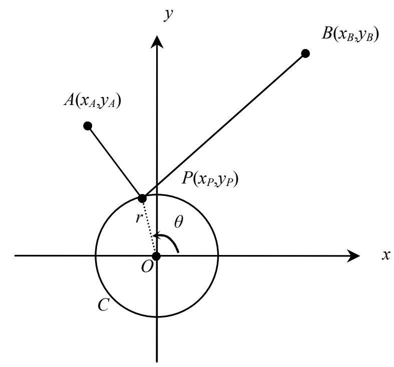

Figure 3. An example of the Q_1^2 problem.

Chou [8] introduced the difficulties of resolving the general root formula, and proposed a method which is taking advantage of the law of light reflection in physics [10-13] and fundamental geometry [14-16] to find the optimal P which yields the shortest path of the Q_1^2 problem. The shortest traversal length L can be rewritten as

$$L = \min\{\ell(\theta_1), \ell(\theta_2), \ell(\theta_3), \ell(\theta_4), \ell(\theta_5), \ell(\theta_6), \ell(\theta_7), \ell(\theta_8)\} \quad (3)$$

where

$$\theta = \begin{cases} \theta_1 = -\cos^{-1}(\frac{1}{4}k - n - \frac{1}{2}\sqrt{q-p}) \\ \theta_2 = \cos^{-1}(\frac{1}{4}k - n - \frac{1}{2}\sqrt{q-p}) \\ \theta_3 = -\cos^{-1}(\frac{1}{4}k - n + \frac{1}{2}\sqrt{q-p}) \\ \theta_4 = \cos^{-1}(\frac{1}{4}k - n + \frac{1}{2}\sqrt{q-p}) \\ \theta_5 = -\cos^{-1}(\frac{1}{4}k + n - \frac{1}{2}\sqrt{q+p}) \\ \theta_6 = \cos^{-1}(\frac{1}{4}k + n - \frac{1}{2}\sqrt{q+p}) \\ \theta_7 = -\cos^{-1}(\frac{1}{4}k + n + \frac{1}{2}\sqrt{q+p}) \\ \theta_8 = \cos^{-1}(\frac{1}{4}k + n + \frac{1}{2}\sqrt{q+p}), \end{cases}$$

where

$$k = \frac{r(ax_B + bx_A)}{ab}$$

$$n = \frac{1}{2}\sqrt{\frac{l}{2} + \frac{1}{j}(\frac{g}{h} + h)}$$

$$p = \frac{m}{8a^3b^3n}$$

$$q = l - \frac{1}{j}(\frac{g}{h} + h),$$

where $a, b, c, d, e, f, g, h, j, l, m$ are

$$a = x_A^2 + y_A^2$$

$b = x_B^2 + y_B^2$

$c = 2r^2 x_A x_B + r^2 y_A^2 + x_B^2(r^2 - 4y_A^2) + 2r^2 y_A y_B + r^2 y_B^2 - 4y_A^2 y_B^2 + x_A^2(r^2 - 4b)$

$d = 2x_A^2 x_B + x_B y_A(y_A - y_B) + x_A(2x_B^2 - y_B(y_A - y_B))$

$e = x_B^2(-r^2 + y_A^2) - 2x_A x_B(r^2 - y_A y_B) + x_A^2(-r^2 + y_B^2)$

$f = 36r^2(6e(ax_B + bx_A)^2 + cd(ax_B + bx_A) + 6abd^2)$

$g = c^2 + 48abe + 24r^2 d(ax_B + bx_A)$

$h = \frac{1}{\sqrt[3]{2}} \sqrt[3]{2c^3 - 288abce + 2f + \sqrt{-4g^3 + 4(c^3 - 144abce + f)^2}}$

$j = 12ab$

$l = -\frac{c}{3ab} + \frac{r^2(ax_B + bx_A)^2}{2a^2b^2}$

$m = r(r^2(ax_B + bx_A)^3 - abc(ax_B + bx_A) - 4a^2b^2d).$

Chou [8] had shown the correctness of (3) in that paper, we conclude by the following theorem.

Theorem 2. *Equation* (3) *can compute the shortest path of a* Q_1^2 *problem.*

IV. ALGORITHM

To sum up all the details above mentioned, this section generalizes an exact algorithm to immediately computing the shortest path of three spheres and is thus facilitating for programming. The algorithm begins with a loop of iterations three, due to there are three combinations of the traversal order as mentioned in the beginning of Section 2. In each iteration, we first shift the three spheres making the center of the middle sphere coincided with the origin. After computing the equation of plane E and the equation of line ζ which is the intersection of plane E and xy-plane, angles ϕ and φ are obtained accordingly, which are the included angles about line ζ and x-axis and plane E and xy-plane respectively. The algorithm is now sufficient to rotate xy-plane making it coincided with plane E to reduce the problem from a 3D space system to a corresponding 2D space system. To achieve this, we first CCW rotate about z-axis for ϕ degree, this generates a new coordinates system from xyz to $x'y'z'$. We further CCW rotate about x'-axis for φ degree, this creates another new coordinates system from $x'y'z'$ to $x''y''z''$. Now the $x''y''$-plane is completely stuck on plane E. All points on plane E have an identical z''-axis value "0".

The algorithm enters the core procedure for computing the optimal P in a reduced Q_1^2 problem with two points and one circle. By applying (3), the optimal P'' is immediately obtained by selecting the smallest values from the eight roots. The problem is now resolved in a 2D system, however we have to restore all results back to their original 3D system. The restore steps are similar to that of the rotation steps just described by simply taking the inversed transition matrices instead of all the original transition matrices. The last step is to shift back all the restored results to their original positions to finish one loop. After all three loops of three traversal orders completed in this manner, the algorithm outputs the shortest path from among the three computed paths. We have the following algorithm.

Algorithm Shortest_Path(S_A, S_B, S_C, $path_{\min}$, $L_{\min}$)
Input : S_A as S_1, S_B as S_2 and S_C as S_3.
Output : The shortest path $path_{\min}$ and its length $L_{\min}$.

path()={null}; $path_{\min}$ ={null}; //initialization
$L_{\min}$ =∞;
For (*j*=1; *j*<=3; *j*++;)
{
Shift the center of S_j to the origin and re-compute the coordinates of the center of each sphere;
Compute the equation of plane E based on the three centers;
Compute the intersection of plane E and xy-plane, which is line ζ;
Compute the included angle of ζ and x-axis, which is ϕ;
Compute the included angle of plane E and xy-plane, which is φ;
Applying (1) to CCW rotate about z-axis for ϕ degree and then CCW rotate about x'-axis for φ degree; //this generates the coordinates system from xyz-system to $x'y'z'$-system and then $x''y''z''$-system.
Applying equation (3) about the general root formula of the reduced Q_1^2 problem obtaining the optimal point P'';
Applying equation (2) to CW rotate about x''-axis for φ degree and then CW rotate about z'-axis for ϕ degree to obtain the results (including P'') to the original xyz-system; //this restores the coordinates system from $x''y''z''$-system to $x'y'z'$-system and then xyz-system;
Shift back all the results (including P) to the original location;
Add the other two contact points (point A and point B for example) on the first and the last spheres and P to the set of *path*(*j*) and compute the length of *path*(*j*) as *L*(*j*);
if *L*(*j*)< $L_{\min}$ {
$L_{\min}$= *L* (*j*);
$path_{\min}$=*path*(*j*);}
}
Return $path_{\min}$ and $L_{\min}$;

V. EXAMPLE

We will show an example to thoroughly go through the proposed algorithm in this section. The computational precision of the example follows the IEEE 754 eight bytes double precision floating point specification [17] which is an accurate signed 16 digits decimal system. Three spheres S_A, S_B, and S_C with their centers O_A(-30,25,20), O_B(25,20,15), and O_C(-5,4,-4) respectively, and their corresponding radii r_A =2, r_B =4, and r_C =8. Under this traversal order $S_A - S_C - S_B$ for the illustration of the first loop, we first shift all three spheres by $(x+30, y-25, z-20)$ making the center of S_C coincided with the origin. We get three new centers denoted as O_{A*}(-25,21,24), O_{B*}(30,16,19), and O_{C*}(0,0,0). The co-plane E can be computed by the three points as

$$\begin{vmatrix} x-(-25) & y-21 & z-24 \\ 0-(-25) & 0-21 & 0-24 \\ 30-(-25) & 16-21 & 19-24 \end{vmatrix} = 0 .$$

We get the equation of the co-plane

$$E\colon \; -15x - 1195y + 1030z = 0 .$$

The included angle φ of co-plane E and xy-plane, and the included angle ϕ of x-axis and line ζ can be obtained by the following equations

$$\varphi = -\cos^{-1}\left(\frac{1030}{\sqrt{(-15)^2 + (-1195)^2 + (1030)^2}}\right)$$

and

$$\phi = \cos^{-1}\left(\frac{1}{\sqrt{1 + \left(\frac{-(-15)}{-1195}\right)^2}}\right) .$$

We get φ=-0.8594589315648351 and ϕ=0.01255164206956715. The other two angles are $\pi - \varphi$ and $\pi - \phi$. By applying equation (1), which rotates about z-axis for ϕ degree and then rotates about x'-axis for φ degree which comes out the coordinates of O_A'' (-25.26160829187317, 31.68361006116514, 0) and O_B'' (29.79681587524359, 25.08285796508905, 0).

Now that the z''-axis of the two points O_A'' and O_B'' are all equal to 0, we can concentrate on solving the reduced Q_1^2 problem with two points O_A'', O_B'' and one circle C_C. By applying (3) we immediately obtain the optimal contact point P'' in the middle circle C_C with P''(0.8165224257906952, 7.958221605872815, 0). We then start the restore processes to map P'' back to its original P in the original coordinates system as follows. By applying equation (2), we first CW rotate x''-axis about φ degree and then CW rotate about z'-axis for ϕ degree, we get

P(0.8816685072409563, 5.184846739645711, 6.028268816975960).

With shifting the coordinates by $(x-30, y+25, z+20)$, we have the exact coordinates of

P(-4.118331492759044, 9.184846739645711, 2.028268816975960). in its original spherical surface.

By connecting segments $\overline{O_A P}$ and $\overline{O_B P}$, we have the two intersections P_A(-28.53177311318545, 24.10283090020072, 18.98049158159424) and P_B(21.53988661800658, 18.71484200481173, 13.45857717963118) locating on S_A and S_B respectively. Then we have three contact points P_A, P and P_B locating on S_A, S_C and S_B respectively which yields the length of $\left|\overline{P_A P}\right| + \left|\overline{P_B P}\right|$ = 62.91738771466268 which is the minimum. The remaining two loops generate the lengths of the other two traversal orders $S_A - S_B - S_C$ and $S_B - S_A - S_C$ with the lengths of 77.12309892316599 and 80.28622021887737 respectively.

We use a brute force method for comparison. The brute force method is to randomly select arbitrary one point on the surface of each sphere and then computes the length of the two interconnecting links according to the traversal order used in the proposed algorithm, say, $S_A - S_C - S_B$ to complete one iteration. As far as the iteration grows, the random selection finds shorter and shorter paths. However, according to our experiments, until the iteration goes to 10^7, we have a shortest path 62.9173922489587 among these 10^7 iterations which is still a certain gap to our result under a requested computational precision. This comparison method is also to identify the correctness and the effectiveness of the proposed algorithm.

VI. CONCLUSION

In this paper, the problem of finding the Euclidean shortest path of three spheres in 3D space is to be degenerated to the corresponding problem of finding the Euclidean shortest traversal path of a three coplanar circles problem in 2D plane and then reduced to a Q_1^2 problem. Our previous work had shown that although the reduced Q_1^2 problem is simple in its appearance, the intrinsic complexity is not that straightforward and cannot resolve the general roots formula by applying traditional methods. In the inspiration by Snell's law in light reflection, our previous work had resolved the general root formula of the Q_1^2 problem. We then propose an exact algorithm which comprises all the details of the degenerations of the problem and the core computation of the Q_1^2 problem to immediately compute the shortest path of three spheres. After demonstrating an example and in contrasting with a brute force method, the algorithm displays its correctness and performance so that it is applicable for computer systems. As to the more general problem of traversing n spheres in 3D space, this paper provides the base model of n=3. Developing an efficient algorithm of finding the shortest traversal path of n spheres in 3D space is our future work which is still essentially open.

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