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A New Fast Direct Solution to the Problem of the Sphere Tangent to Four Spheres

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Abstract

A simple non-iterative process to solve in 2D, 3D and hyperspaces the problem of the tangency of spheres is presented and proved. Solutions are obtained immediately with high numerical precision.

Finding the sphere tangent to four others is important in crystallography, especially to develop theoretical models of structures. The problem of the location and size of cations between structural units or layers has been described elsewhere as the *VOID* program (Langlet, Figueiredo & Lima-de-Faria, 1977).

Several iterative solutions have been proposed in the past (Mackay, 1973; Sickafus & Mackie, 1974; Langlet, 1977).

A general mathematical treatment of the problem (Hocquemiller, 1977) gave for the first time the possibility of obtaining a direct solution so that we experimented with success in computer programs written in Fortran as well as in APL.

The new solution presented here only requires a 3 × 3 matrix inversion instead of a 4 × 4 one in 3D, and therefore can be easily applied on pocket calculators.

Let T be a square matrix with the following organization:

$$\mathbf{T}=\begin{pmatrix} r_1 & x_1 & y_1 & z_1 \cdots \\ r_2 & x_2 & y_2 & z_2 \cdots \\ r_3 & x_3 & y_3 & z_3 \cdots \\ r_4 & x_4 & y_4 & z_4 \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{1}$$

r_i, x_i, y_i, z_i are respectively the radius and the center coordinates of sphere i. The dots correspond to further coordinates in the columns of **T** and to further hyperspheres in the rows of **T** for n-dimension spaces.

In 3D, **T** is a 4 × 4 matrix, then in nD, **T** is a $(n+1)\times(n+1)$ matrix.

The general formula to find the coordinates $r, x, y, z, \cdots$ of the sphere tangent to $(n+1)$ ones is:

$$(x-x_i)^2+(y-y_i)^2+(z-z_i)^2+\cdots-(r+r_i)^2=0, \tag{2}$$

with $i=1, 2, \cdots n+1$.

The system of $n+1$ equations has $n+1$ unknown parameters: $r, x, y, z, \ldots$

Equations (2) may be developed:

$$-r^2+x^2+y^2+z^2+\cdots-2[rr_i+xx_i+yy_i+zz_i+\cdots]$$

$$-r_i^2+x_i^2+y_i^2+z_i^2\ldots=0 \tag{3}$$

Subtracting equations $i+1$ from equations i one obtains n equations:

$$r(r_i-r_{i+1})+x(x_i-x_{i+1})+y(y_i+y_{i+1})+z(z_i-z_{i+1})$$
$$=\tfrac{1}{2}[(r_i^2-r_{i+1}^2)+(x_{i+1}^2-x_i^2)+(y_{i+1}^2-y_i^2)$$
$$+(z_{i+1}^2-z_i^2)]. \tag{4}$$

This system is linear, but since it still has $n+1$ unknown parameters, let us write it in matrix notation as a function of r:

$$\mathbf{MV}=\mathbf{S}+\mathbf{P}r, \tag{5}$$

where **M** is the matrix

$$\begin{pmatrix} x_1-x_2 & y_1-y_2 & z_1-z_2\cdots \\ x_2-x_3 & y_2-y_3 & z_2-z_3\cdots \\ x_3-x_4 & y_3-y_4 & z_3-z_4\cdots \\ \vdots & \vdots & \vdots \end{pmatrix},$$

i.e. a 3 × 3 matrix in 3D, and **V**, **S**, **P** are the following column vectors:

$$\mathbf{V}=\begin{pmatrix} x \\ y \\ z \end{pmatrix},\quad \mathbf{P}=\begin{pmatrix} r_2-r_1 \\ r_3-r_2 \\ r_4-r_3 \end{pmatrix},$$

$$\mathbf{S}=\tfrac{1}{2}\begin{pmatrix} (r_1^2-r_2^2)+(x_2^2-x_1^2)+(y_2^2-y_1^2)+(z_2^2-z_1^2) \\ (r_2^2-r_3^2)+(x_3^2-x_2^2)+(y_3^2-y_2^2)+(z_3^2-z_2^2) \\ (r_3^2-r_4^2)+(x_4^2-x_3^2)+(y_4^2-y_3^2)+(z_4^2-z_3^2) \end{pmatrix},$$

the solution of equation (5) will be:

$$\mathbf{V}=\mathbf{M}^{-1}\mathbf{S}+\mathbf{M}^{-1}\mathbf{P}r, \tag{6}$$

then:

$$\underline{\mathbf{V}}=\underline{\mathbf{S}}+\underline{\mathbf{P}}r, \tag{7}$$

with $\underline{\mathbf{S}}=\mathbf{M}^{-1}\mathbf{S}$ and $\underline{\mathbf{P}}=\mathbf{M}^{-1}\mathbf{P}$.

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One will immediately notice that the coordinates of the center of the sphere are a linear function of its radius and may be computed easily with a 3 × 3 matrix inversion only, when R is known.

So, let us introduce (7) into any of the equations (2) with the following notation:

$$\mathbf{V}_i = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix}.$$

Equation (2) becomes:

$$(\mathbf{V} - \mathbf{V}_i)^2 - (r + r_i)^2 = 0. \tag{8}$$

Let us develop (8) and replace $\mathbf{V}$ by its expression (7)

$$\bar{\mathbf{V}}^2 - 2\mathbf{V}.\,\mathbf{V}_i + \bar{\mathbf{V}}_i^2 - (r + r_i)^2 = 0. \tag{9}$$

Then,

$$\bar{\underline{\mathbf{S}}}^2 + 2\underline{\mathbf{S}}.\underline{\mathbf{P}}r + \bar{\underline{\mathbf{P}}}^2 r^2 - 2\mathbf{V}_i(\underline{\mathbf{S}} + \underline{\mathbf{P}}r) + \bar{\mathbf{V}}_i^2 - r^2 - 2rr_i + r_i^2 = 0 \tag{10}$$

or

$$(\bar{\underline{\mathbf{P}}}^2 - 1)r^2 + 2(\underline{\mathbf{S}}\underline{\mathbf{P}} - \underline{\mathbf{P}}\mathbf{V}_i - r_i)r + \bar{\underline{\mathbf{S}}}^2 - 2\underline{\mathbf{S}}\mathbf{V}_i + \bar{\mathbf{V}}_i^2 - r_i^2 = 0, \tag{11}$$

$$(\bar{\underline{\mathbf{P}}}^2 - 1)r^2 + 2[\underline{\mathbf{P}}(\underline{\mathbf{S}} - \mathbf{V}_i) - r_i]r + (\underline{\mathbf{S}} - \mathbf{V}_i)^2 - r_i^2 = 0. \tag{12}$$

Let us call $\mathbf{D}$ the difference

$$\mathbf{S} - \mathbf{V}_i. \tag{13}$$

Then, r is one of two solutions of the second degree equation, the coefficients of which are:

$$\begin{aligned} a &= \bar{\underline{\mathbf{P}}}^2 - 1, \\ b' &= \underline{\mathbf{P}}.\mathbf{D} - r_i, \\ c &= \bar{\underline{\mathbf{D}}}^2 - r_i^2. \end{aligned} \tag{14}$$

$\Delta = b'^2 - ac$ must be ≥ 0, the solution $(-b' + \sqrt{\Delta})/a$ stands for the radius of the sphere externally tangent and the solution $(-b' - \sqrt{\Delta})/a$ for the sphere internally tangent, the one that will interest crystallographers.

Now, (7) immediately yields $\mathbf{V}$, *i.e.* x, y, z, ..., as a linear function of r.

So, with simple expressions only using a 3 × 3 matrix inversion in 3D, one can get the direct solution on a pocket calculator, or even by hand, knowing that if one also includes a transformation matrix from oblique coordinates to Cartesian ones, the whole solution from the original crystal cell only requires 3 × 3 matrices.

All the formulae here remain valid in 4D, 5D, *etc.* spaces. Formal calculation is also possible so as to obtain expressions as functions of the radii.

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   LET T BE AN ARRAY ACCORDING TO (1)
G←(−Q[;1]),0 1↓Q←T×T
S←0.5×+/⁻1 0↓G−1⊖G
P←⁻1↓(1⌽T[;1])−T[;1]
M←⌹M←⁻1 0↓U−1⊖U←0 1↓T
   (M IS THE INVERSE OF MATRIX M)
S←M+.×S
P←M+.×P
VI←1↓T[1;]
RI←T[1;1]
D←S−VI
A←+/⁻1,P×P
BP←(D+.×P)−RI
C←(D,RI)+.×D,−RI
Δ←(BP×BP)−A×C
   THEN, IF Δ≥0
R←((−BP)−Δ*0.5)÷A
V←S+P×R
   ACCORDING TO (7)

THE SIGN ⌹(DOMINO) IS ÷AND □SUPERIMPOSED
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Fig. 1. APL demonstration (and computing program).

APPENDIX

The powerful Iverson's (1962) notation APL provides a good way of repeating the demonstration in a concise way (Fig. 1). This formulation is at the same time the whole computing program that may be assembled into a pair of APL expressions and provides a good guide for programming in any other language such as Fortran or Basic.

Moreover, several problems may be solved simultaneously since APL works on high rank arrays without explicit loops: one can invert at the same time several 3 × 3 matrices by pure indexing of their components; this has led us to write very small APL programs for mini-computers (available upon request) to find at once all the voids – location and size of interstitial sites – among a whole set of packing atoms. The only limitation comes from the workspace size, due to the combinatory process involved.

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