E11-2002-296

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FAST ANALYTICAL METHOD FOR COMPUTING VOLUME OF OVERLAPPING SPHERES

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1 Introduction

Solvent environment plays a crucial role on the structure and function of biological macromolecules, such as DNA, RNA and proteins. Exact determination of direct interactions between the macromolecules and the solvent molecules still remains a very hard mathematical and computational problem. By this reason a different kinds of approximations are usually done which allow to describe these extremely complicated interactions through physically averaged macroscopic parameters. Such an effective parameters are, for example, solvent accessible area of the solute molecule and the so called excluded volume. Computation of these parameters requires evaluation of complicated algorithms. For this reason, any effort to development an effective analytical methods is always welcomed.

Richmond [1] has defined the solvent-excluded volume to mean the volume contained within the solvent accessible surface, i.e. the volume which is inaccessible to the centers of solvent particles. That is the union of the expanded atom spheres. The excluded volume is an important quantity in the theory of gases and liquids [2]. The exploration of molecular volume and surface is essential for the understanding of drug action since short range dispersion forces play a major role in the binding of drug molecules to receptors (`http://server.ccl.net/cca/documents/molecular-modeling`).

The problem of the computation of volume of the union of overlapping spheres has been the subject of methods both numerical (Rowlinson, 1963; Pavani and Ranghino, 1982; Gavezzotti, 1983) and analytic (Richmond, 1984; Kang, Nemethy and Scheraga, 1987; Gibson, and Scheraga, 1987a; Gibson, and Scheraga, 1987b; Gibson, and Scheraga, 1988; Guerrero-Ruiz, Ocadiz-Ramirez and Garduno-Juarez, 1991; Petitjean, 1994) (see `http://www.netsci.org/Science/Compchem/feature14g.html`).

At `http://www.biohedron.com/bibliography.html` one can find references to this topic.

In this paper two exact analytical methods for the calculation of the volume of overlapping spheres are described. This methods evolve the approach utilized by authors of [3] for surface area calculation. In the considered procedure the volume of the system of overlapping spheres is expressed by surface integrals over closed region. Using the stereographic projection (see [4]) of the sphere surface points onto a plane tangent to the atom and opposite the origin located at spheres North Pole, particular surface integrals are transformed to double integrals which are further reduced to the curve integrals. A different way of using the stereographic projection for molecular surface calculation was described in [5].

2 The Method

We describe the molecule S as a union of the spheres (atoms) $S_1, \ldots, S_n$ (see fig 1). Hence $S = \bigcup_{j=1}^{n} S_j$. Let (x_i, y_i, z_i) be Cartesian coordinates of the center of the i-th sphere and r_i be the radius of this sphere, where $1 \leq i \leq n$. For $j \neq i$ we say that S_j is *a neighbor of* S_i if $\text{in}\,(S_i) \cap \text{in}\,(S_j) \neq \emptyset$, where $\text{in}\,(S)$ denotes the interior of the set S.

The algorithm of volume computation can be briefly presented as

Volume integral $\Longrightarrow$ Surface integral $\Longrightarrow$ Double integral $\Longrightarrow$ Line integral

We shall compute volume $V(S)$ by using Gauss-Ostrogradsky's theorem which allows to reduce the volume $V(S)$ evaluation to the surface integrals of the second kind

$$V(S) = \iiint_S dx\,dy\,dz = \iint_{B(S)} z\,dx\,dy = \sum_{i=1}^{n} \iint_{B_i(S)} z\,dx\,dy, \qquad (1)$$

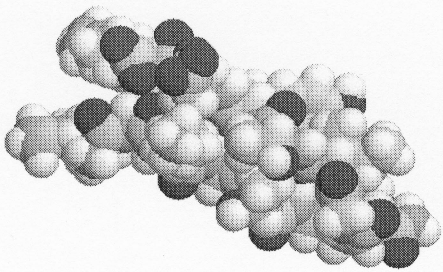

Figure 1: Visualization of the molecular surface

where $B(S)$ is the surface of S and $B_i(S)$ is as a part of surface of S_i which is **outside of all its neighbors**. All integrals at right side of (1) can be calculated separately. At this point the problem of computing $V(S)$ is reduced to computing n surface integrals.

Next step is the transformation of the surface integral over the particular surface $B_i(S)$ to the double integral. This can be done by transformation of the surface $B_i(S)$ onto the tangent (to the South Pole of S_i) plane.

2.1 Stereographic projection

The points (x, y, z) of the i-th sphere's surface satisfy the equation

$$(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 = r_i^2. \tag{2}$$

The equations

$$\begin{aligned} x &= x_i + 4r_i^2 t/(t^2 + s^2 + 4r_i^2) \\ y &= y_i + 4r_i^2 s/(t^2 + s^2 + 4r_i^2) \\ z &= z_i + r_i - 8r_i^3/(t^2 + s^2 + 4r_i^2) \end{aligned} \tag{3}$$

describe a projection of the points of the i-th sphere's surface from its *North*

Pole point (NP) onto the plane $(t, s) \in \mathbb{R}^2$, tangent to the sphere at the *South Pole*. This is a one-to-one map except the point $(x_i, y_i, z_i + r_i)$ (NP).

The equations

$$\begin{aligned} t &= -2r_i(x - x_i)/(z - z_i - r_i) \\ s &= -2r_i(y - y_i)/(z - z_i - r_i) \end{aligned} \tag{4}$$

express the inverse transformation.

The points which are not inside the j-th sphere satisfy the following inequality

$$(x - x_j)^2 + (y - y_j)^2 + (z - z_j)^2 \geq r_j^2. \tag{5}$$

On the other hand, the points of the i-th sphere's surface which are outside of the j-th sphere or on its surface, satisfy Eq. (2) and Eq. (5). Transformation of those points to the (t, s) plane using Eq. (3) leads to

$$a_j^i(t^2 + s^2) + b_j^i t + c_j^i s + d_j^i \geq 0, \tag{6}$$

where

$$\begin{aligned} a_j^i &= (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i + r_i - z_j)^2 - r_j^2 \\ b_j^i &= 8r_i^2(x_i - x_j) \\ c_j^i &= 8r_i^2(y_i - y_j) \\ d_j^i &= 4r_i^2\left[(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - r_i - z_j)^2 - r_j^2\right]. \end{aligned} \tag{7}$$

Let us denote by Ω_i the set of the points on (t, s) plane which correspond to $B_i(S)$ by the stereographic projection. Define $\Psi_i = \{j;\ S_j$ is a neighbor of $S_i\}$. So, Ψ_i is a set of indices of neighbors of S_i. Then

$$\Omega_i = \{(t, s);\quad a_j^i(t^2 + s^2) + b_j^i t + c_j^i s + d_j^i \geq 0 \text{ for all } j \in \Psi_i\}. \tag{8}$$

Since (6) represents either interior of a circle ($a_j^i < 0$) or exterior of a circle ($a_j^i > 0$) or half plane ($a_j^i = 0$) then Ω_i is an intersection of those parts of (t, s) plane (see figure 2). It is easy to see that if S_i has no neighbors then $\Omega_i = \mathbb{R}^2$ and $B_i(S)$ is the whole surface of S_i and the corresponding surface integral is equal $(4/3)\pi r_i^3$ (the i-th sphere's volume). On the other hand, if the whole *surface of* $S_i \subset \bigcup_{j \in \Psi_i} S_j$ then $B_i(S) = \emptyset$ and $\Omega_i = \emptyset$.

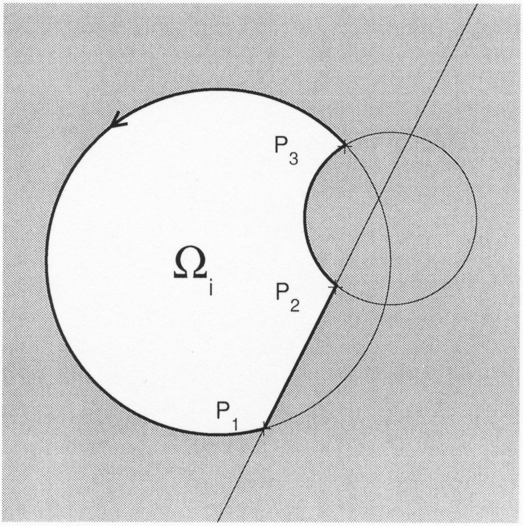

Figure 2: The plane image Ω_i of the surface part $B_i(S)$

2.2 $\iint\limits_{B_i(S)} z\,dx\,dy$ computation

For computing the surface integrals in Eq. (1) we will use the known formula which transforms the surface integral to the double integral. In view of Eq. (3) we have the Jacobian

$$\mathcal{J}_i(t,s) = \begin{vmatrix} \dfrac{\partial x}{\partial t} & \dfrac{\partial x}{\partial s} \\ \\ \dfrac{\partial y}{\partial t} & \dfrac{\partial y}{\partial s} \end{vmatrix}$$

$$\mathcal{J}_i(t,s) = 16r_i^4 \frac{4r_i^2 - t^2 - s^2}{(t^2+s^2+4r_i^2)^3}.$$

Consequently,

$$\begin{aligned} \iint\limits_{B_i(S)} z\,dx\,dy &= -\iint\limits_{\Omega_i} \left\{ z_i + r_i - \frac{8r_i^3}{t^2+s^2+4r_i^2} \right\} \mathcal{J}_i(t,s)\,dt\,ds \\ &= 128r_i^7 \iint\limits_{\Omega_i} \left\{ \frac{\partial Q(t,s)}{\partial t} - \frac{\partial P(t,s)}{\partial s} \right\} dt\,ds \stackrel{\text{def}}{=} \mathcal{I}_i \end{aligned} \tag{9}$$

where

$$Q(t,s) = \frac{t}{3(t^2+s^2+4r_i^2)^3} + \frac{t}{192r_i^4(t^2+s^2+4r_i^2)} + \frac{t}{(t^2+s^2+4r_i^2)^2}\left[\frac{1}{48r_i^2} - \frac{z_i+r_i}{16r_i^3}\right],$$

$$P(t,s) = \frac{-s}{3(t^2+s^2+4r_i^2)^3} + \frac{-s}{192r_i^4(t^2+s^2+4r_i^2)} + \frac{-s}{(t^2+s^2+4r_i^2)^2}\left[\frac{1}{48r_i^2} - \frac{z_i+r_i}{16r_i^3}\right].$$

At first, we assume that Ω_i is **bounded**. Then applying Green's theorem to Eq. (9) we transform the double integral to the curve integrals in the following way

$$\mathcal{I}_i = \frac{128r_i^7}{3}\oint\limits_{B(\Omega_i)} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)^3} + \frac{2r_i^3}{3}\oint\limits_{B(\Omega_i)} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)} - \frac{8r_i^4(3z_i+2r_i)}{3}\oint\limits_{B(\Omega_i)} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)^2},$$

where $B(\Omega_i)$ is the boundary of Ω_i. Therefore, $B(\Omega_i)$ is generated by points of (t,s) plane satisfying

$$a_j^i(t^2+s^2) + b_j^i t + c_j^i s + d_j^i = 0, \quad \text{for some } j \in \Psi_i. \tag{10}$$

Eq. (10) describes either a circle ($a_j^i \neq 0$) or a line ($a_j^i = 0$). Hence, $B(\Omega_i)$ consists of parts of circles or parts of lines. It is easy to see that $a_j^i = 0$ geometrically corresponds to the situation when the surface of j-th sphere passes through the *North Pole* of the i-th sphere.

2.3 $\oint\limits_{B(\Omega_i)} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)^k}$ computation

Let $N_i \subset \Psi_i$ be the set of order numbers of the spheres which intersect the i-th sphere, and Λ_j^i be the number of arcs which generate the boundary of Ω_i and descend from the j-th sphere and all arcs $C_{j,\lambda}^i$ together form the boundary of Ω_i. $C_{j,\lambda}^i$ are oriented positively with respect to Ω_i when $a_j^i < 0$ and negatively, otherwise. Each arc $C_{j,\lambda}^i$ is part of a circle or a line. Then we have

$$\oint\limits_{B(\Omega_i)} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)^k} = \sum_{j\in N_i}\sum_{\lambda=1}^{\Lambda_j^i} \oint\limits_{C_{j,\lambda}^i} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)^k}, \quad k=1,2,3. \quad (11)$$

In order to simplify the formulas we will omit the upper index i further in the text everywhere, except the cases when it may cause misunderstanding. To compute the volume $V(S)$, it is sufficient to give formulas for the following curve integrals:

$$J_k = \oint\limits_{C_{j,\lambda}} \frac{t\,ds - s\,dt}{(t^2+s^2+4r_i^2)^k}, \qquad k=1,2,3.$$

There are two possibilities. If $C_{j,\lambda}$ is the circlular arc given by Eq. (10) (where $a_j \neq 0$) then $C_{j,\lambda}$ is parametrized as follows:

$$\begin{aligned} t &= t_0 + r_0\cos\varphi \\ s &= s_0 + r_0\sin\varphi \end{aligned} \qquad \text{for} \quad \varphi \in \langle \alpha_{j,\lambda};\beta_{j,\lambda}\rangle. \quad (12)$$

After some computations we arrive to the following relations.

$$J_1 = \frac{\beta_{j,\lambda} - \alpha_{j,\lambda} + (r_0^2 - A)I_1}{2},$$

$$J_2 = \frac{I_1 + (r_0^2 - A)I_2}{4}, \quad J_3 = \frac{I_2 + (r_0^2 - A)I_3}{8},$$

where

$$I_k = \int\limits_{\alpha_{j,\lambda}}^{\beta_{j,\lambda}} \frac{d\varphi}{(A + B\cos\varphi + C\sin\varphi)^k}, \qquad k=1,2,3$$

with

$$B = t_0 r_0, \quad C = s_0 r_0, \quad A = \frac{4r_i^2 + t_0^2 + s_0^2 + r_0^2}{2}$$

and

$$t_0 = -\frac{b_j}{2a_j}, \quad s_0 = -\frac{c_j}{2a_j}, \quad r_0 = \sqrt{\frac{b_j^2 + c_j^2 - 4a_j d_j}{4a_j^2}}.$$

If we denote

$$D = A^2 - B^2 - C^2$$

then one can verify that for the case when $\beta_{j,\lambda} - \alpha_{j,\lambda} < 2\pi$ the following formulas hold

$$I_1 = \frac{2}{\sqrt{D}} \left[\frac{\pi}{2} - \arctan \frac{A\cos^- + B\cos^+ + C\sin^+}{\sqrt{D}\sin^-} \right],$$

where

$$\cos^- = \cos\frac{\beta_{j,\lambda} - \alpha_{j,\lambda}}{2}, \qquad \cos^+ = \cos\frac{\alpha_{j,\lambda} + \beta_{j,\lambda}}{2},$$

$$\sin^+ = \sin\frac{\alpha_{j,\lambda} + \beta_{j,\lambda}}{2}, \qquad \sin^- = \sin\frac{\beta_{j,\lambda} - \alpha_{j,\lambda}}{2},$$

$$I_2 = \frac{1}{A^2 - B^2 - C^2} \left[\left. \frac{-B\sin x + C\cos x}{A + B\cos x + C\sin x} \right|_{\alpha_{j,\lambda}}^{\beta_{j,\lambda}} + A\, I_1 \right],$$

$$I_3 = \frac{1}{2D} \left[\left. \frac{-B\sin x + C\cos x}{(A + B\cos x + C\sin x)^2} \right|_{\alpha_{j,\lambda}}^{\beta_{j,\lambda}} + \left. \frac{\frac{-B}{A}\sin x + \frac{C}{A}\cos x}{A + B\cos x + C\sin x} \right|_{\alpha_{j,\lambda}}^{\beta_{j,\lambda}} \right] + \frac{2A^2 + B^2 + C^2}{2A\,D} I_2.$$

For the case when $\beta - \alpha = 2\pi$ the integrals I_1, I_2, I_3 are equal:

$$I_1 = \frac{2\pi}{D^{1/2}}, \qquad I_2 = \frac{2\pi A}{D^{3/2}}, \qquad I_3 = \frac{\pi(2A^2 + B^2 + C^2)}{D^{5/2}}.$$

For I_k there exist explicit formulas (see, for example, [6]).

Now we consider the second case, namely the extreme situation when $C_{j,\lambda}$ is a line segment with the start point $A = \langle t_0, s_0 \rangle$ and the end point $B = \langle t_1, s_1 \rangle$. In view of Eq. (10) let us assume that $C_{j,\lambda}$ lies on the line $b_j t + c_j s + d_j = 0$. Then we can describe $C_{j,\lambda}$ as follows

$$\begin{aligned} t &= t_0 + k\, c_j \cdot \varphi \\ s &= s_0 - k\, b_j \cdot \varphi \end{aligned} \qquad \text{for} \quad \varphi \in \langle 0; 1 \rangle, \tag{13}$$

where $k = (t_1 - t_0)/c_j = -(s_1 - s_0)/b_j$. In this case

$$J_1 = \frac{k\, d_j}{C} \tilde{I}_1, \qquad J_2 = \frac{k\, d_j}{C^2} \tilde{I}_2,$$

$$J_3 = \frac{k\, d_j}{4(AC - B^2)} \left[\frac{B + C}{(C + 2B + A)^2} - \frac{B}{A^2} + \frac{3}{C} \tilde{I}_2 \right],$$

where

$$\widetilde{I}_1 = \frac{C}{\sqrt{AC - B^2}} \left[\arctan \frac{B + C}{\sqrt{AC - B^2}} - \arctan \frac{B}{\sqrt{AC - B^2}} \right],$$

$$\widetilde{I}_2 = \frac{C^2}{2(AC - B^2)} \left[\frac{B + C}{C + 2B + A} - \frac{B}{A} + \widetilde{I}_1 \right]$$

with

$$A = 4r_i^2 + t_0^2 + s_0^2, \quad B = k(c_j t_0 - b_j s_0), \quad C = b_j^2 + c_j^2.$$

In the case when Ω_i is unbounded, but $\Omega_i^c = \mathbb{R}^2 - \Omega_i$ is bounded we can use the following equality

$$16r_i^4 \iint\limits_{\Omega_i} \left[\frac{\partial Q(t,s)}{\partial t} - \frac{\partial P(t,s)}{\partial s} \right] dt\, ds + \\ + 16r_i^4 \iint\limits_{\Omega_i^c} \left[\frac{\partial Q(t,s)}{\partial t} - \frac{\partial P(t,s)}{\partial s} \right] dt\, ds = \frac{4}{3}\pi r_i^3,$$

for computing of surface integral in Eq. (9).

When both regions Ω_i and Ω_i^c are unbounded then

$$\lim_{r \to \infty} \int\limits_{C(r)} \frac{t\, ds - s\, dt}{t^2 + s^2 + 4r_i^2} = \gamma, \quad \lim_{r \to \infty} \int\limits_{C(r)} \frac{t\, ds - s\, dt}{(t^2 + s^2 + 4r_i^2)^j} = 0, \quad j = 2, 3, \tag{14}$$

where $C(r)$ is a positively oriented circle part with the fixed center point accordant to the radius r and the angle γ.

Let $C_{j,\lambda}$ be the half line segment with starting point (t_0, s_0) which lies on the line $p:\ b_j t + c_j s + d_j = 0$. Denote

$$A = 4r_i^2 + t_0^2 + s_0^2, \quad B = k(c_j t_0 - b_j s_0), \quad C = b_j^2 + c_j^2$$

and

$$I_1 = \frac{C}{\sqrt{AC - B^2}} \left[\frac{\pi}{2} - \arctan \frac{B}{\sqrt{AC - B^2}} \right].$$

Then

$$J_1 = \frac{k\, d_j}{C} I_1, \qquad J_2 = \frac{k\, d_j}{2(AC - B^2)} \left[I_1 - \frac{B}{A} \right], \\ J_3 = \frac{k\, d_j}{4(AC - B^2)} \left[\frac{3C}{2(AC - B^2)} \left(I_1 - \frac{B}{A} \right) - \frac{B}{A^2} \right], \tag{15}$$

where $k = 1$ in the case when the orientation of half line is in direction of vector $(c_j, -b_j)$ and $k = -1$ in the case when the orientation of half line is in direction of vector $(-c_j, b_j)$.

Remark 1 *Using the rotations of the whole molecule one can avoid the case of straight lines boundary parts of Ω_i. In this case, the boundary of Ω_i or Ω_i^c consists only of circular arcs, and Ω_i or Ω_i^c is bounded.*

Remark 2 *Following [3], the surface area of the overlapping spheres is*

$$A = \sum_{i=1}^{n} \left[\chi(\Omega_i) + 2r_i^2 \sum_{j \in N_i} \sum_{\lambda=1}^{N_j} \int_{C_{j,\lambda}} \frac{t\,ds - s\,dt}{t^2 + s^2 + 4r_i^2} \right],$$

where

$$\chi(\Omega_i) = \begin{cases} 0, & \Omega \text{ is bounded,} \\ 4\pi r_i^2, & \Omega \text{ is all plane except several rings,} \\ 2r_i^2\gamma, & \Omega \text{ is an angle of size } \gamma \text{ with some picked bounded part} \end{cases}$$

and can be calculated together with the volume using formula for J_1.

3 Partial volume computation

In this section we deal with separate volume computation of "free part" of some atom. In other words, let S_1 be arbitrary sphere. Denote by S_2, $\ldots$, S_k, all nontrivial neighbors of S_1. Let $F = S_1^{2,\ldots,k}$ denote the part of S_1 which is **outside of all its neighbors** S_2, $\ldots$, S_k. We shall compute volume $V(F)$. Gauss-Ostrogradsky theorem allows to reduce volume $V(F)$ to the surface integrals

$$\begin{aligned} V(F) &= \iiint\limits_{F} dx\,dy\,dz = \iint\limits_{B(F)} (z - z_1 - r_1)\,dx\,dy \\ &= \iint\limits_{B_1(F)} (z - z_1 - r_1)\,dx\,dy + \sum_{\ell=2}^{k} \iint\limits_{B_\ell(F)} (z - z_1 - r_1)\,dx\,dy \end{aligned} \tag{16}$$

where $B(F)$ is the surface of F and $B_1(F)$ is a part of surface of S_1 which is **outside of its neighbors** $S_2, \ldots, S_k$ and $B_\ell(F)$, $\ell = 2, \ldots, k$ is defined as a part of surface of S_ℓ, which is **inside** S_1 **and outside of all other neighbors of** S_1.

3.1 Computation of the integral $\iint\limits_{B_\ell(F)} (z - z_1 - r_1)\,dx\,dy$

We will use the above described stereographic projection method to compute the surface integrals in Eq. (16).

$$\begin{aligned}\iint\limits_{B_1(F)} (z - z_1 - r_1)\,dx\,dy &= 128r_1^7 \iint\limits_{\Omega_1} \frac{4r_1^2 - t^2 - s^2}{(t^2 + s^2 + 4r_1^2)^4}\,dt\,ds \\ &= 128r_1^7 \iint\limits_{\Omega_1} \left[\frac{\partial Q(t,s)}{\partial t} - \frac{\partial P(t,s)}{\partial s}\right] dt\,ds\end{aligned} \tag{17}$$

where in this case

$$Q(t,s) = \frac{t}{3(t^2 + s^2 + 4r_1^2)^3} + \frac{t}{48r_1^2(t^2 + s^2 + 4r_1^2)^2} + \frac{t}{192r_1^4(t^2 + s^2 + 4r_1^2)},$$

$$P(t,s) = \frac{-s}{3(t^2 + s^2 + 4r_1^2)^3} + \frac{-s}{48r_1^2(t^2 + s^2 + 4r_1^2)^2} + \frac{-s}{192r_1^4(t^2 + s^2 + 4r_1^2)}.$$

Let us Assume that Ω_1 is bounded. Then the Green's theorem for transformation of the double integral to the curve integral applied to Eq. (17) yields

$$\iint\limits_{B_1(F)} (z - z_1 - r_1)\,dx\,dy = \frac{128r_1^7}{3} \oint\limits_{B(\Omega_1)} \frac{t\,ds - s\,dt}{(t^2 + s^2 + 4r_1^2)^3} +$$
$$\frac{8r_1^5}{3} \oint\limits_{B(\Omega_1)} \frac{t\,ds - s\,dt}{(t^2 + s^2 + 4r_1^2)^2} + \frac{2r_1^3}{3} \oint\limits_{B(\Omega_1)} \frac{t\,ds - s\,dt}{(t^2 + s^2 + 4r_1^2)},$$

where $B(\Omega_1)$ is the boundary of Ω_1. Similarly,

$$\iint\limits_{B_\ell(F)} (z - z_1 - r_1)\,dx\,dy = \iint\limits_{B_\ell(F)} (z - z_\ell - r_\ell)\,dx\,dy + (z_\ell - z_1 + r_\ell - r_1) \iint\limits_{B_\ell(F)} dx\,dy$$

for $\ell = 2, \ldots, k$. To compute $\iint\limits_{B_\ell(F)} (z - z_\ell - r_\ell)\, dx\, dy$ we can proceed as above. Consequently, using Eq. (3) with $i = \ell$ one gets

$$\iint\limits_{B_\ell(F)} (z - z_\ell - r_\ell)\, dx\, dy = \frac{128 r_\ell^7}{3} \oint\limits_{B(\Omega_\ell)} \frac{t\, ds - s\, dt}{(t^2 + s^2 + 4r_\ell^2)^3} + \frac{8 r_\ell^5}{3} \oint\limits_{B(\Omega_\ell)} \frac{t\, ds - s\, dt}{(t^2 + s^2 + 4r_\ell^2)^2} + \frac{2 r_\ell^3}{3} \oint\limits_{B(\Omega_\ell)} \frac{t\, ds - s\, dt}{(t^2 + s^2 + 4r_\ell^2)},$$

where $B(\Omega_\ell)$ is boundary of Ω_l. On the other hand,

$$\iint\limits_{B_\ell(F)} dx\, dy = \iint\limits_{\Omega_\ell} 16 r_\ell^4 \frac{4r_\ell^2 - t^2 - s^2}{(t^2 + s^2 + 4r_\ell^2)^3} dt\, ds = 8 r_\ell^4 \oint\limits_{B(\Omega_\ell)} \frac{t\, ds - s\, dt}{(t^2 + s^2 + 4r_\ell^2)^2}.$$

One can easily see, that in this case the above written formulas may be used to calculate J_k, too. The case of unbounded domain Ω_i is solved in a similar way.

Remark 3 *The described method for calculation of the partial volume may be useful when we add to the molecule with known volume one new atom. In this case we can compute its "free volume", which will be the volume change of the whole molecule.*

Remark 4 *After computing the "free volume" of the first atom S_1, we can delete this atom from the list of the spheres, and go on with computation of the "free volume" of some other atom, and so on. This way we can compute the whole volume of the system of overlapping spheres.*

4 Numerical results

In this section we briefly describe numerical results for some "molecules". Three data sets were used for this purpose. First and second (see Eq. (18)) contain 3, resp. 7 spheres, the third one contains 295 atoms.

We compared the results of our analytical method with the results from a numerical method (which is most likely not the best one). All calculations are done on SPP'2000 machine. We failed to compare the performance of our program with other analytical algorithms because we don't have any at hand by now.

	Analytical method	Division number in numerical method		
		10^3	20^3	100^3
3 atoms	$1 \cdot 10^{-4}$ s 211.7957	$7 \cdot 10^{-4}$ s 210 0.0084	$5.3 \cdot 10^{-3}$ s 214.2 0.01135	$1.2 \cdot 10^{-1}$ s 211.809 $6.45 \cdot 10^{-5}$
7 atoms	$5.2 \cdot 10^{-3}$ s 211885.361	$1.6 \cdot 10^{-3}$ s 20151.936 0.079	$1.2 \cdot 10^{-2}$ s 21781.872 0.0047	$6.7 \cdot 10^{-1}$ s 21901.006 $7.15 \cdot 10^{-4}$
295 atoms	$3.6 \cdot 10^{-1}$ s* 2769.388	$5.4 \cdot 10^{-2}$ s 2769.071 $1.14 \cdot 10^{-4}$	$4.3 \cdot 10^{-1}$ s 2769.071 $1.14 \cdot 10^{-4}$	52 s 2768.678 $2.56 \cdot 10^{-4}$

* $3.6 \cdot 10^{-1}$ s on 600Mhz/256MB RAM Pentium
$1.9 \cdot 10^{-1}$ s on 1.8Ghz/512MB RAM AMD AthlonXP

Table 1: Comparison of numerical with proposed analytical method

$$\begin{matrix} 0 & 0 & 0 & 3 \\ 4 & 0 & 0 & 3 \\ 0 & 3 & 0 & 1 \end{matrix} \qquad \begin{matrix} 0 & 0 & 0 & 2 \\ 11 & 0 & 0 & 10 \\ -11 & 0 & 0 & 10 \\ 0 & 11 & 0 & 10 \\ 0 & -11 & 0 & 10 \\ 0 & 0 & 11 & 10 \\ 0 & 0 & -11 & 10 \end{matrix} \tag{18}$$

Corresponding first rows in each section of the table 1 contain computation time in seconds, second rows contain the computed volume and third rows contain relative error of "numerical results".

5 Conclusion

We can see from table 1 that the proposed analytical method is faster than numerical method with sufficient points density. It can successfully run on parallel computers. The computation time of simultaneous calculation surface area and volume is practically the same as the time for volume computation only.

This work was supported by the RFBR 02-01-00606

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Received on December 28, 2002.

Айрян Э. А. и др. E11-2002-296
Быстрый аналитический метод вычисления объема
перекрывающихся шаров

Предложен точный аналитический метод расчета общего объема перекрывающихся шаров. В рассмотренной процедуре объем выражается как поверхностный интеграл второго рода по замкнутой поверхности. При использовании стереографической проекции этот интеграл преобразуется в сумму двойных интегралов и далее в сумму криволинейных интегралов.

После небольших изменений предложенный метод может быть использован для расчета частичного «свободного» объема отдельного шара.

Работа выполнена в Лаборатории информационных технологий ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна, 2002

Ayrjan E. A. et al. E11-2002-296
Fast Analytical Method for Computing Volume
of Overlapping Spheres

An exact analytical method for the calculation of volume of overlapping spheres is presented. In the considered procedure the volume is expressed as a surface integral of the second kind over the closed region. Using the stereographic projection the surface integral is transformed to a sum of double integrals which are reduced to curve integrals.

Slightly modified, this method can be used for calculation of a partially «free» volume of a separated sphere.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna, 2002

Макет *Т. Е. Попеко*

Подписано в печать 31.01.2003.
Формат 60 × 90/16. Бумага офсетная. Печать офсетная.
Усл. печ. л. 1,18. Уч.-изд. л. 1,75. Тираж 310 экз. Заказ № 53741.

Издательский отдел Объединенного института ядерных исследований
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