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***Abstract*— An interesting property of the Voronoi tessellation is studied in the context of its application to the analysis of hydration shells in computer simulation of solutions. Namely the shells around a randomly chosen cell in a Voronoi tessellation attract extra volume from outside. There is a theoretical result which says that the mean volume of the first shell around a randomly chosen cell is greater than the anticipated value. The paper investigates this phenomenon for Voronoi tessellations constructed for computer models of point patterns with different variability of the Voronoi cell volumes (Poisson point process, RSA systems of hard spheres and molecular dynamics models of water). It analyzes also the subsequent shells, and proposes formulas for the mean shell volumes for all shell numbers. The obtained results are of value in calculations of the contribution of hydration of water to the "apparent" volume of the solutes.**

Keywords- Voronoi tessellation; topological neighbors; shell volume; solvation shell

I. INTRODUCTION

It is an established opinion that the structure of water close to a solute molecule differs from the structure in pure or bulk water (at some distance from the solute) [1]. The charge of an ion or the size of a neutral molecule influences the mutual arrangement of the water molecules close to the solute molecule. This "hydration water" may have a lower or higher density, depending on the solute. The investigation of hydration water plays an important role in molecular biology. It governs the folding-unfolding process of proteins. The "apparent" volume of solutes depends on hydration water. The addition of a solute molecule to water results in a difference V^{app} between the volumes of the prepared solution and the volume of the water content as pure liquid. The measurement of the apparent volume is a task of experimental research and computer simulations in physical chemistry of solutions, in particular for the interpretation of the results of volumetric experiments in molecular biology [2-5].

The apparent volume may be divided in two parts: $V^{app} = V^{int} + \Delta V^{water}$. The intrinsic volume V^{int} is the neat volume of the solute molecule, sometimes defined as its van der Waals volume, and ΔV^{water} is the contribution of water, which accounts for a possible difference between the densities of bulk and hydration water. The latter can be written as

$$\Delta V^{water} = V^h - v_0 n^h , \qquad (1)$$

where V^h is the volume occupied by the hydration water molecules, n^h is the number of these molecules, and v_0 is the mean volume of a water molecule in bulk water [1]. The calculation of ΔV^{water} gives the possibility to separate the contribution of the intrinsic volume V^{int} from the apparent volume.

Formula (1) is general in the sense that the notion "hydration water" is not defined here explicitly. To use this formula, the parameter V^h has to be concretized and the number of solvent molecules n^h has to be known. One of the ways to make it is using the Voronoi diagram technique, which is described in many papers and books, see e.g. [6,7]. In this approach to each atom a cell is assigned, its Voronoi cell. This cell represents a volume belonging to the atom. This approach is very attractive for analysis of computer models of molecular systems and is used for many years [8,9].

However this tool may be more powerful if the cells are considered amounting to the entire Voronoi tessellation decomposing space. Using this tessellation enables to establish topological neighborhoods of the cells (atoms). The nearest neighbors (the first topological neighbors or "the geometrical neighbors") of a given central atom represent the first Voronoi shell around this atom. The next topological neighbors form the subsequent shells. Thus in this approach, hydration water can be determined by the water molecules in the first (or in a few of the closest) Voronoi shells around the solute molecule.

To our knowledge there are only a few papers where such a description of hydration water has been used. Only the first Voronoi shell was considered in the papers [10-12], the first and second ones were discussed in paper [13]. Another approach is based on the simple idea to determine hydration water by a layer of given thickness R around the solute molecule. However, there is uncertainty to choose the value of R, and a difficulty to estimate the possible error of the calculated volume of hydration water. In spite of this, the method is used in many papers, see in particular [4,5,14]. By the way, sequences of shells have also been studied in the 2D

case for the structural analysis of patterns, polycrystals and foams, where some topological laws of the tessellation were found and investigated [15-17].

When the authors began to use Voronoi shells in the volumetric analysis of hydration water, an interesting observation was made: the shell volumes turned out to be a bit larger than expected. This fact was first observed by Weiss [18] for the first shell. It seems that the set of cells in a shell is not a representative subset of a tessellation. In the present paper we study this phenomenon systematically, based on computer simulations for various systems of atoms. This leads to formulas for a more accurate calculation of the contribution of hydration water ΔV^{water} to the apparent volume of solutes.

II. THE FIRST SHELL

It is well known that for the case of a completely random point system (a Poisson process of points) a randomly chosen Voronoi cell has on average f = 15.54 faces. The mean number of faces changes if instead of a randomly chosen cell a volume weighted cell is considered. The corresponding mean value f^w is calculated by $\sum v_i f_i / \sum v_i$, where v_i and f_i are the volume and the number of faces of the i-th cell. It can be shown that f^w = 16.577, i.e. the value is somewhat larger than f. This may be plausible since in some sense the volume weighted cell is larger than a randomly chosen one and the number of faces and the volume of Poisson Voronoi cells are positively correlated [19-20].

The difference between f^w and f depends on the disorder of the system. As it will be shown below for Voronoi tessellations of our systems, it holds

$$\left(f^w - f\right)/f \propto \sigma^2/v_0^{\,2}, \qquad (2)$$

where v_0 is the mean volume of the typical Voronoi cell and σ^2 is the variance of its volume. The results of computer simulations carried out by the authors confirm the validity of (2), see Table 1 and Fig.1.

The quantity f^w appears in the following formula (3), which seems to be unexpected. Let V_1 be the mean volume of the first shell around a randomly chosen cell. Weiss [18] has shown that

$$V_1 = v_0 f^w. \qquad (3)$$

One could perhaps think that it should be $V_1 = v_0 f$. Indeed, the first shell contains in average just f cells, and the mean cell volume is v_0. However, the situation is more complicated, the random variables "cell volume" and "number of faces" are not independent.

Since $f^w > f$ the shell contains some extra volume. A possible explanation is that there are generating points that contribute to the shell, which are far from the central cell and possess cells with large volumes. In other words, far "geometrical neighbors" of the central point have on average cell volumes greater than v_0.

Let us to introduce "the mean volume of a cell inside the first shell" by $v_1 = V_1 / f$. (The authors are aware that they do not use a quite correct terminology. The mean volume of a cell inside the shell is mathematically defined a bit differently by considering the random numbers of cells in shell. By the way, these two means coincide very well as a special calculation carried out by the authors has shown). Using the parameter v_1, formula (3) can be rewritten as

$$v_1 = v_0 f^w / f \qquad (4)$$

Note that the volume V_1 (and accordingly v_1) could be obtained explicitly by calculation of cell volumes in shells. The Weiss formula gives another possibility, namely to calculate it using the topological characteristics (f and f^w).

Table 1 shows numerical values for the discussed characteristics obtained by simulation for various models. Model 1 is a system of 512,000 random points in a cubic box with periodic boundary conditions. The edge of the box is equal to 80 length units, which implies that the mean cell volume is v_0=1. The models 2 - 4 are systems of centers of 500,000 random monodisperse non-overlapping spheres of radii 0.2, 0.25 and 0.3 correspondingly, obtained by the RSA (random sequential adsorption) approach, see [21]. These points are also in a cubic box with periodic boundary conditions. The box edge is again chosen to ensure v_0=1 for the mean volume of the corresponding Voronoi cells. The different radii were used in order to obtain different variances of the Voronoi cell volumes distributions. The models 5 - 6 are usual molecular dynamic models of pure water with different temperatures and constant density. Such water models are used as solvents in molecular biology and physical chemistry simulations [3,4]. Every sample consists of 10,000 water molecules, which are considered for the Voronoi analysis as points centered at the oxygen atoms.

For every model the Voronoi tessellation was calculated. The numbers of faces and volumes for all Voronoi cells were

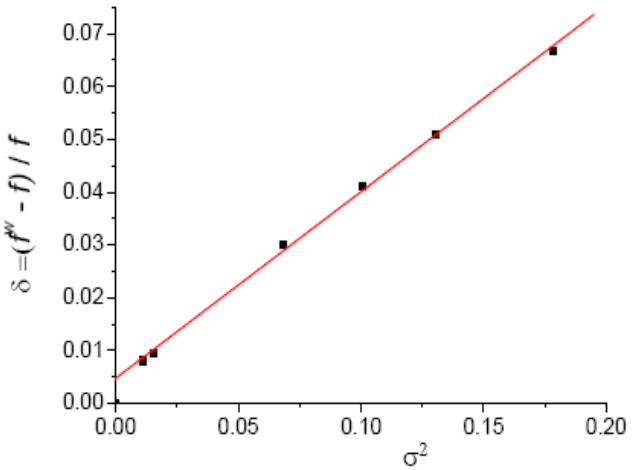

Figure 1. Parameter $\delta = (f^w - f)/f$ for the various models as a function of the variance of the Voronoi cell volume

TABLE I. AVERAGE CHARACTERISTICS OF THE FIRST SHELL FOR THE STUDIED MODELS.

Model	f	f^w	f^w/f	v_0	σ^2	V_1	v_1
1. Poisson	15.536	16.573	1.06676	1	0.1782	16.5685	1.06628
2. RSA 0.20	15.500	16.289	1.05091	1	0.1304	16.3043	1.05169
3. RSA 0.25	15.447	16.084	1.04124	1	0.1007	16.0891	1.04115
4. RSA 0.30	15.377	15.840	1.03008	1	0.0681	15.8224	1.03023
5. Water 280K	15.921	16.049	1.00804	29.825A^3	3.170612 0.01130	30.0645	1.00802
6. Water 490K	15.221	15.367	1.00956	29.825A^3	3.680857 0.01523	30.1107	1.00957

The mean number of cell faces f, the number of faces f^w for the volume weighted cell, their ratio, the mean volume of the typical cell v_0, the variance of cell volume σ^2, the mean volume V_1 of the first shell, and the mean volume v_1 of the cells in the first shell. In the last two lines in the 6-th column both the true and normalized mean volumes are presented.

determined and used to obtain the mean values in Table 1. The mean values for the Poisson and RSA models are obtained by averaging over 50,000 randomly chosen central cells. For the water models the averaging was performed over 999 independent configurations of a molecular dynamics simulation run of water, using 1000 water molecules in every configuration as central cells.

The very good coincidence of the numbers in the fourth and last columns confirms the validity of formula (4) for all models considered. Remember that the values f^w/f in the fourth column are obtained from topological information, whereas the metric values V_1 and v_1 in Table 1 are calculated directly from the cell volumes.

Fig. 1 demonstrates the behavior of the parameter $\delta = (f^w - f) / f$ as a function of the variance of the Voronoi cell volume for our models. We see a linear behavior as predicted in formula (2). However, our line does not go through the origin though one can think that the value δ should be zero at $\sigma^2 = 0$. This means that the behavior of δ via σ^2 may be more complicated than predicted by formula (2).

III. THE SUBSEQUENT SHELLS

Fig. 2 illustrates a series of subsequent shells around a single cell in 2D. Such shells are well defined in the Voronoi tessellation: the cells of the k-th shell have common faces with cells of the (k-1)-th shell and are not adjacent to cells of the previous shells. In this section we will analyze the subsequent shells in our 3D models discussed above.

Let n_k be the mean number of cells belonging to the k-th shell, and V_k be the mean total volume of the k-th shell, which is determined as the sum of volumes of the shell's cells. The mean volume v_k of the cells inside the k-th shell is defined as V_k/n_k.

We now study the value v_k in dependence on shell number k. Fig. 3 shows results obtained for the models considered. (Note, working with many shells, the averaging was made only for 5000 typical cells). One can see that the mean cell volume v_k has a maximum value for the first shell (k=1), decreases then systematically with growing k, and converges towards the mean volume of a single cell v_0.

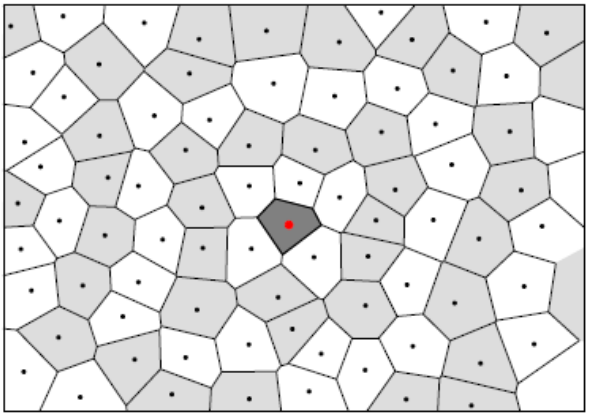

Figure 2. 2D illustration of the Voronoi tessellation of a system of points shown as dots. Shells around the central cell are marked. The cells belonging to the k-th shell are the k-th topological neighbors of the central cell (with a red point).

Note it is always $v_k > v_0$, which looks strange from a naive point of view. Indeed, if one would try to calculate the mean volume of a single cell for the whole system based on the shells then a result greater then v_0 would be obtained, as long as k is finite. A possible explanation for this behavior was already given in the context of discussion of formulas (3) and (4). Now we see that not only the first shell but also the other shells are able to attract extra volumes from outside.

It is possible to develop an approximation formula which gives the mean cell volume v_k for any k-th shell for Voronoi tessellations, thus to generalize formula (4), which holds for the first shell. To do this, let us assume that any face of a cell is able to attract some extra volume. In other words, the mean volume v_i of the cell adjacent to the i-th face of a given cell is greater than v_0. As mentioned above, this is possible if some far geometrical neighbors have mean cell volumes larger than v_0. Thus one can write $v_i = v_0\gamma$, where the factor $\gamma = 1+\delta$ is greater than 1, and δ is a small correction term.

Using the factor γ, the mean volume of the first shell V_1 can be written as

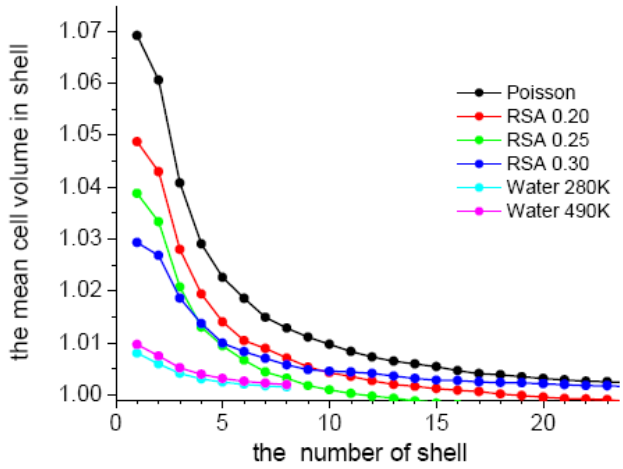

Figure 3. Mean cell volume v_k in shells as a function of shell number k calculated for the models discussed in section 2.

$$V_1 = n_1 v_0 \gamma \,. \tag{5}$$

Comparison with formula (3) yields

$$\gamma = f^w / f \tag{6}$$

and

$$\delta = \left(f^w - f\right)/f \,. \tag{7}$$

Assuming that γ is a universal factor for all faces of all cells of the tessellation, we can determine the mean volume of the second shell as

$$V_2 = n_2 v_0 \gamma - n_1 v_0 \delta \,.$$

The first term is the total volume "attracted" by the outer faces of the first shell. (Note that the number of the outer faces of the first shell determines the number of cells in the second shell). The second term takes into account the fact that some extra volume attracted to the first shell had been involved at the expense of the second shell and must be subtracted. This formula can be rewritten as $V_2 = n_2 v_0 \gamma_2$, where

$$\gamma_2 = 1 + \delta\left(1 - n_1/n_2\right).$$

For the mean cell volume in the second shell defined as $v_2 = V_2 / n_2$, we get:

$$v_2 = v_0 \gamma_2 \,.$$

The same reasoning may be used also for the following shells. Thus we obtain

$$v_k = v_0 \gamma_k \,, \tag{8}$$

with

$$\gamma_k = 1 + \delta\left(1 - n_{k-1}/n_k\right), \tag{9}$$

where δ is given by formula (7), and $k > 1$.

It is useful to have an asymptotic formula for γ_k which does not depend on the values n_{k-1} and n_k. Such a formula can be derived by assuming that the number n_k is proportional to the surface area of the k-th shell. The surface is roughly spherical and its area is approximately proportional to the square of its radius. The radius of the k-th sphere can be estimated as kD, where D is a scale parameter (a "diameter") of the cells, which is a constant for a given tessellation. Thus $n_{k-1}/n_k \sim (k-1)^2/k^2$, which gives:

$$\gamma_k^{asympt} = 1 + 2\delta/k - \delta/k^2 \,. \tag{10}$$

One can see that both formulas for the γ_k factors (asymptotic (10) and initial (9)) give very close values for prediction of the v_k values, see Fig. 4.

IV. Applications

As we have seen, shells attract extra volume from outside. This means that in the analysis of hydration water by Voronoi tessellations we should take into account this phenomenon to calculate the correct contribution of water in the apparent volume ΔV^{water}, see also the introduction.

The mean volume assigned to n_k independent molecules in bulk water is $v_0 n_k$. However if they constitute a Voronoi shell this value should be corrected by the factor γ_k, i.e. it is equal to $v_0 n_k \gamma_k$. Thus, if one presents the volume of hydration water as a sum of volumes of the nearest Voronoi shells $V^h = V_1 + V_2 + V_3 + \ldots$, the formula for the calculation of ΔV^{water} can be written as:

$$\begin{aligned} \Delta V^{water} = {} & V_1 - v_0 n_1 \gamma + \\ & + V_2 - v_0 n_2 \gamma_2 + \\ & + V_3 - v_0 n_3 \gamma_3 + \ldots \end{aligned} \tag{11}$$

Fig. 4 helps to estimate the value of the correction factor γ_k. For unit mean volume ($v_0 = 1$), Fig.4 presents directly the values of γ_k. For Poisson points the correcting factor for the first shell is about 7%, for the next shells it is smaller, but up to the 10-th shell it is still larger than 1%. For water, which is more important in physical applications, the effect is smaller because the variance of the Voronoi cell volumes in water is smaller, see Table 1 and Fig.1. This yields for the first shell γ = 1.0080, for the second γ_2 = 0.00603, for the third γ_3 = 0.00447 for water at 280K.

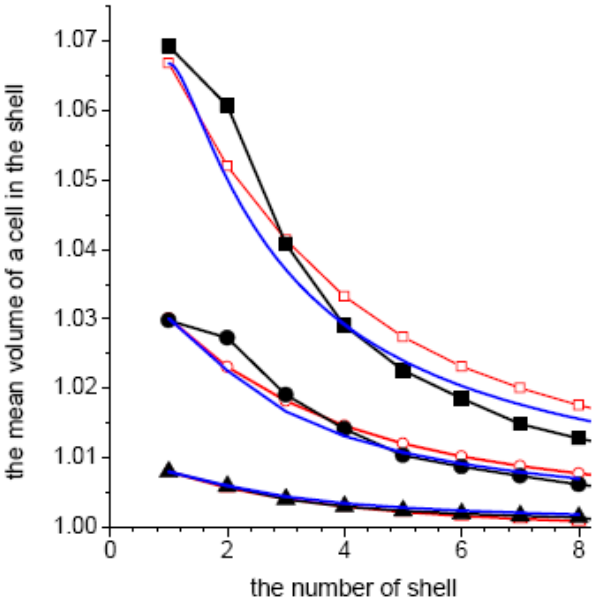

Figure 4. Values of v_k as a function of shell number k for Poisson points (upper curves, squares), for the model RSA 0.30 (mid curves, circles), and for the water model at 280K (lower curves, triangles). Shown are the values taken from Fig. 3 (black, large symbols), and those predicted by formula (8) (red, small symbols) and (10) (blue, lines)

However, these estimations are not yet useful for real solutions, since they are obtained for shells around a single cell. In real solutions a solute molecule can be rather large. Then the first shell of the solute contains a larger number of Voronoi cells n_1^{solute} than a single Voronoi cell, see Fig.5. Using the formula (5) we can write:

$$V_1^{solute} = n_1^{solute} v_0 \gamma . \qquad (12)$$

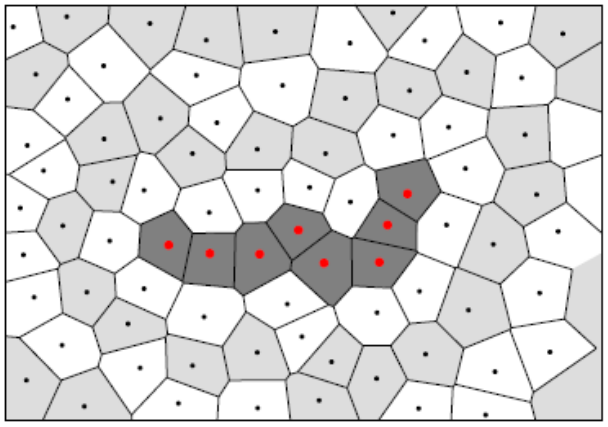

Figure 5. 2D illustration of Voronoi shells around a large "solute molecule" (a cluster of cells wit red points in the center). The cells of the k-th shell are the k-th topological neighbors of the cells of the "solute molecule".

For the other shells we can also obtain formulas similar to (8) and (9):

$$V_k^{solute} = n_k^{solute} v_0 \gamma_k^{solute} \qquad (13)$$

with

$$\gamma_k^{solute} = 1 + \delta\left(1 - n_{k-1}^{solute} / n_k^{solute}\right). \qquad (14)$$

Here the value δ correspond to the pure solvent, however the values n_k^{solute} depend on the solute studied.

We estimated values of γ_k^{solute} for the molecular dynamics model of a polypeptide water solution simulated in [22]. We found the mean numbers n_1^{solute} = 332, n_2^{solute} = 513 and n_3^{solute} = 775. They yield γ_2^{solute} = 1.0028 and γ_3^{solute} = 1.0027 for δ = 0.008. For the first shell obviously $\gamma_1^{solute} = \gamma$ =1 + δ= 1.0080, see (12).

Thus for larger solute molecules the γ - factors for the far shells becomes smaller than for a single cell, see (9). However for the first shell it is the same as for a single central cell.

V. Conclusion

In this paper we investigated the Voronoi shells around a given cell in a Voronoi. tessellation. The work was motivated by the unexpected property of the shells to have mean volumes larger than the mean volume of the same number of cells distributed independently. Ignoring this property may have undesirable consequences in applications of the Voronoi method to analyze the solvation shells in computer models of solutions.

We analyzed successive shells in models containing around 500,000 disordered points obtained by the Poisson process and by the RSA method to get different variations of the Voronoi cell volume. We have shown that all shells "attract" extra volume from outside, and this value depends on the variability of the point systems: the effect decreases with decrease of variations of the cell volume.

The mean volume of a cell inside the k-th shell v_k (reciprocal density of the shell) has a maximum value for the first shell (k=1), and decreases with growing k converging towards the mean volume of a single cell v_0. At that $v_k > v_0$ for all k. This fact looks strange from a naive point of view. It indicates that the set of cells in the shell is not a representative subset of the tessellation.

Simple formulas for estimation of extra volume attached to the k-th shell were presented. They can be used for the investigation of solvation shells in computer models of solutions, in particular, for the calculation of the contribution of hydration water to the "apparent" volume. Important for such studies, the analysis of computer models of liquid water shows a small effect (less then a percent) for water solutions. This results from rather small variations of the Voronoi cells in water in comparison with a model based on a Poisson point process.

Note that formula (3) is mathematically exact, whereas our generalization (formulas (9) and (14)) is only a result of

heuristic approximations. The authors hope that this paper will encourage mathematicians to create a rigorous theory of mean shell volumes in tessellations.

ACKNOWLEDGMENT

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