Computer program simulation of protein structure and theory of mechanic force for protein folding II

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ABSTRACT

In the previous paper [21], we have worked out the calculation of the coordinates of the atoms in polypeptide chain, and the mathematical procedures for computing the coordinates of atoms of the alpha helices and 3^{10} helices, based on the deterministic theory of atomic structure.

In this paper, we work out the computer programs to carry out the calculation and the computer graphics of the primary structure and the secondary helix structure of proteins.

We elaborate on the arguments for theory of mechanic force for protein folding into a secondary and tertiary structure.

We also work out the rotation and the calculation in computer graphic program to orient the computer generated helix segment to coincide with the helix segment in the tertiary structure of proteins based on experiment. We need only the coordinates of two proper points in the helix segment from the experiment to orient the computer generated helix segment.

Keywords: Computer graphic program, Deterministic theory of atomic structure, Protein structure, Numerical coordinates, Theory of mechanic force for protein folding.

1 INTRODUCTION

Quantum mechanics is probabilistic, and cannot provide the precise structures of atoms. If we apply Maxwell equation directly to atomic structure, the atom will radiate and becomes unstable. Therefore, we assume that Maxwell equation can not apply to atomic structure. We need to modify the Maxwell equation to account for the stable atomic structure. The deterministic theory of atomic structure consists of a set of Electrodynamic Equations applicable to atomic structures. Their mathematical solution provides definite stable orbits for electrons to move around the nucleus of atoms and molecules.

The set of Electrodynamic Equations is following:

$$\nabla \times E = -\frac{\mu}{c}\frac{\partial H}{\partial t}$$

$$\nabla \times H = 0$$

$$\nabla \cdot E = 0$$

$$\nabla \cdot H = 0$$

Their mathematical solution in spherical coordinate (r, θ, φ, t) is following:

$$\phi_l^m(r,\theta,\varphi,t) = cosC_1 t Y_l^m(\theta,\varphi) r^{\frac{-1}{2}} J_{l+\frac{1}{2}}(C_1\frac{\mu}{c}r)$$

where $\phi_l^m(r,\theta,\varphi,t)$ is the electric potential, $Y_l^m(\theta,\varphi)$ is the spherical harmonics, $J_{l+\frac{1}{2}}(C_1\frac{\mu}{c}r)$ is the Bessel function, l is a positive integer and m is an integer between $-l$ and l, C_1 is a constant.

Based on the deterministic theory of atomic structure, we derive the electronic configurations for atoms, the rules for atoms to joint together to form covalent bonds and hydrogen bonds.

We list few samples of electronic configurations:

$$H:$$

$$l=1, m=0, J_{\frac{3}{2}}^{(1)}; 1e$$

$$C: Gasio-Carbon$$

$$l=1, m=0, J_{\frac{3}{2}}^{(1)}; 2e$$

$$l=2, m=0, J_{\frac{5}{2}}^{(1)}; 2e$$

$$l=3, m=0, J_{\frac{7}{2}}^{(1)}; 2e$$

$$C: Bio-Carbon$$

$$l=1, m=0, J_{\frac{3}{2}}^{(1)}; 2e$$

$$l=3, m=0, J_{\frac{7}{2}}^{(1)}; 2e$$

$$l=3, m=\pm 3, J_{\frac{7}{2}}^{(1)}; \tilde{\theta}=30°or150°; 2e$$

$$O: Bio-Oxygen$$

$$l = 1, m = 0, J^{(1)}_{\frac{3}{2}}; 2e$$

$$l = 2, m = 0, J^{(1)}_{\frac{5}{2}}; 2e$$

$$l = 3, m = 0, J^{(1)}_{\frac{7}{2}}; 2e$$

$$l = 3, m = \pm 3, J^{(1)}_{\frac{7}{2}}; \tilde{\theta} = 30^{\circ} or 150^{\circ}; 2e$$

The rules for forming Bonds are:

- The angular momentum l's of the orbits for sharing electrons are the same.
- The two joining orbits are coplanar.
- The two joining orbits are figure 8 orbit.
- The polarities of the two atoms should be alternating.

In previous paper[21], we provided a brief introduction to the deterministic theory of atomic structure. We produced the numerical coordinate for each atom in a polypeptide chain, and the mathematical steps for the winding of a polypeptide chain to an alpha helix and 3^{10} helix. We also proposed a mechanical force model of the secondary and tertiary structure of proteins.

In this paper, we work out the computer program for calculating the coordinates of each atom in a polypeptide chain and in an alpha helix. We also provide the computer graphics of the polypeptide chain and the alpha helix in the computer programs. We explain some of the technical aspects of the computer programs in Section 2 and 3.

We elaborate on the arguments for the theory of mechanic force for protein folding into the secondary and tertiary structure in Section 4.

We also work out a computer program for orienting a computer generated helix segment to its position of functional state based on experiment in Section 5. We require only the measurements of the coordinates of two proper points of the functional helix segment.

2 COMPUTER GRAPHIC PROGRAM FOR THE PRIMARY STRUCTURE

The name of the variable for the coordinates of the atoms in the polypeptide is a four index variable VP(IP, JP, KP, LP).

The first index IP is the label for the segments in the protein structure. This first index identifies the backbone structures for helix segments and the non-helical segments in protein structure. The index IP is the identification index for the helical and the non-helical segments in the protein structure.

The second index JP is the label for the peptides in the protein segment. The third index KP is the label of the atoms in each peptide. There are eight atomic locations in each peptide, where the residue group is represented by the location of its first atom.

The four index LP is the label for the three X, Y and Z-components of the coordinates of each atom.

We input the maximal number of segments IPM, which gives the dimension for IP, and the maximal number of peptides JPM, which gives the dimension for JP.

The dimension for KP is eight and the dimension for LP is three.

We input the segment label IP for calculation of the segment in question, and the number of peptides JP in this segment.

We input the coordinate the atoms the first peptide. Their coordinates are given in previous paper [21]. They are as following: (0,0,0), (0.8661,-0.5,0), (0.8661,-1.5,0), (-0.8661,-0.5,0). (-0.8661,-1.5,0), (-0.8661,0.5,0), (1.7321,0,0),(0.8661,0.5,0). The unit is Angstrom.

We need to replace Y by -Y, since the screen coordinate Y is going downward. Do-loops on the index KP from 1 to 8 and the index LP from 1 to 3 will take in the coordinates of the first peptide.

The coordinates of the atoms the second peptide is a translation of the first peptide along X-axis by 3*0.8661, and Y-axis by 0.5.

The coordinates of the atoms of the odd peptides are translation of the first peptide along the X-axis by 3 * J * 1.7321, where J the index for the odd peptides. A do-loop on J will perform the calculations of the coordinates of the atoms of the third, the fifth and so on peptides.

The coordinates of the atoms of the even peptides are translation of the second peptide along the X-axis by 3 * J * 1.73211, where J is the index for the even peptides. A do-loop on J will perform the calculations of the coordinates of the atoms of the forth, the sixth and so on peptides.

This complete the calculations of the coordinates of each atoms in the peptide segment.

We then provide the computer graphics of the location of the atoms of the peptide segment. The graphic part of the program consists of a scale factor along X-axis, a scale factor along Y-axis, and a translation along X-axis and Y-axis to position the peptide segment in computer screen.

We use small color circles to represent the atoms and line segments between atoms to represent the bonds.

3 COMPUTER GRAPHIC PROGRAM FOR THE HELIX SEGMENT

In previous paper [21], we had calculated the radius of the alpha helix, the pitch angle of the helix, and provided all the mathematical steps for calculating the coordinates of the atoms of an alpha helix segment. The

radius R of the alpha helix is 1.3545. The pitch angle PHI of the helix is ATN(.5029).

In this Section of the computer program we implement the mathematical steps for calculating the coordinates of the atoms of an alpha helix segment.

The axis of the computer generated helix segment is along Y-axis.

We need the backbone structure from Section 1. The first part of the program is a copy of the computation part of the program of the graphics of the primary structure.

We choose the location of the alpha carbon of the first peptide to be (1,0,0) and the primary structure is along the X-axis.

The second part of the program is the computer implement of the mathematical steps indicated in previous paper [21] to calculate the coordinates of the atoms in the helix segment. It consists of inputing the radius of the alpha helix and the pitch angle of the alpha helix, performing rotation of the backbone structure by an amount of the pitch angle, and then winding up of the inclined backbone structure on the cylinder to obtain the alpha helix and hence the coordinates of the atoms of the alpha helix.

The third part is the graphic program to represent the alpha helix on the computer screen. It is similar to the graphic part of the computer graphics program of the backbone structure.

4 THEORY OF MECHANIC FORCE FOR THE TERTIARY STRUCTURE OF PROTEINS

Although the second and tertiary structure of protein is due to the electric interactions among the atoms of the protein and the water molecules, these electric forces are too numerous to analyze theoretically. If we try to analyze the energy of the protein structure to determine its structure, we get too numerous possibilities of protein structures to consider. Besides, we can not be sure that the energy of the functional state of proteins is an optimal state.

Since the Schroedinger equation is derived only from conservation of energy, without considering conservation of momentum, it does not provide information on the direction of motion of the particles involved. For this reason, if we use Schroedinger equation to analyze the motion of the particles involved, we have specified energy level without specifiied direction of motion. Hence, we need to consider all the possible directions that the particles can move. This is the reason why we arrive a large number of possibilities.

We propose a macroscopic mechanical force theory for protein folding. We have a very precise polypeptide structure based on deterministic theory of atomic structure. It takes force to wind up the backbone structure into a helix. Therefore, the peptide unit in the helix structure produces a counter unit force along the axis of the helix and a counter unit shear force about its axis.

The atoms in the residue groups interact with water molecules to produce forces and shears to propel the backbone to conform to secondary and tertiary structure. Each residue group in the helix produce a unit force along the axis of the helix and a unit shear force about its axis. These forces propel the backbone structure to a helix structure and tertiary structure.

The hydrogen bonds between the peptides contribute to a counter unit force and a unit counter shear force in maintaining the helix structure and the tertiary structure.

The equilibrium of these unit forces, unit shears, unit counter forces and unit counter shears in the protein produce the secondary and tertiary structure.

The non-helix segments is due to the hydrogen bond being torn apart.

We need to measure the counter unit forces, counter unit shears of the backbone, unit forces and unit shears of the residue groups, and the counter force and counter shear of the hydrogen bond. There are fifty of them. Once we have measured these forces and shears, we can then analyze and determine theoretically the secondary and the tertiary structures of proteins. We can translate directly from the DNA coding of proteins to their structures.

Before we achieve these measurements, we need to rely on experiment to determine the tertiary structures of proteins.

5 THE COMPUTER GRAPHIC PROGRAM TO ORIENT THE HELIX

In Section 3, we generate the alpha helix along the direction of the Y-axis. We need to orient the generated helix to have the same orientation as the functional state of the protein segment.

The first part of the computer program is a copy of the computer program in Section 2 so that we have a computer generated helix segment.

We need two points C and D across the helix from the experiment to orient the computer generated helix which is along the Y-axis. We calculate the direction of the line jointing the two cross points, and call it the cross line CD. We assume that C should coincide with A, and D should coincide with B, where A and B are two points on the computer generated helix segment. The cross line CD should coincide with a line AB of the computer generated helix segment.

We orient the computer generated helix segment to the direction of the cross line as following: we first

project the cross line CD and the line AB onto the X-Z plane, calculate the angle ANGXZ between, and rotate about Y-axis the computer generated helix to coincide with the direction of the projection of the cross line.

The formulas for rotation of an angle ANGXZ about Y-axis are following:

VP(IP,J,KP,1)=
VP(IP,J,KP,1)*COSANGXZ
-VP(IP,J,KP,3)* SINANGXZ
VP(IP,J,KP,3)
=VP(IP,J,KP,1)*SINANGXZ
+VP(IP,J,KP,3)* COSANGXZ

where VP's are the coordinate variables of the atoms in the helix segment. The do-loops on J and KP will calculate all the coordinates of the atoms in the helix segment.

Let A' and B' be the A and B respectively after above rotation.

Next, we rotate about Z-axis of the above resulted computer generated helix to coincide with the direction of the cross line. We project A'B' and CD onto the XY-plane and calculate the angle ANGXY between them. We then rotate the newly rotated helix by an angle ANGXY about Z-axis. The formulas for calculating the rotation are following:

VP(IP, J, KP, 1)=
VP(IP, J, KP, 1) * COSANGXY
- VP(IP, J, KP, 2) * SINANGXY
VP(IP, J, KP, 2) =
VP(IP, J, KP, 1) * SINANGXY
+ VP(IP, J, KP, 2) * COSANGXY

where VP's are the coordinate variables for the atoms of the newly rotated helix. The do-loops on J and KP will calculate all the coordinates of the atoms in the helix segment.

Let A" be the result of above rotation on A'.

Finally, we translate the resulted computer generated helix segment to the position of functional state. This means translating the resulted computer generated helix segment so that A" and C coincide.

The graphic part of the program is same as in Section 2 and 3. This will display the helix segment in functional state in the computer screen.

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