Tutorial of radii calculation of nanotube and protein by MolAICal

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1. Introduction

In this tutorial, the radii calculations of nanotube and protein are introduced. This tutorial is divided into three parts: nanotube radii calculation, protein radii calculation and advance radii calculation in peptide channel. The advance radii calculation is based on the PDB and PSF files which are produced by the CHARMM force field.

2. Materials

2.1. Software requirement

1) MolAICal: https://molaical.github.io

2) VMD: https://www.ks.uiuc.edu/Research/vmd

2.2. Example files

1) All the necessary tutorial files are downloaded from:
https://github.com/MolAICal/tutorials/tree/master/005-radiiCal

3. Procedure

3.1. Nanotube radii calculation

1) Build nanotube by VMD software: Extensions→Modeling→Nanotube Builder (see Figure 1).

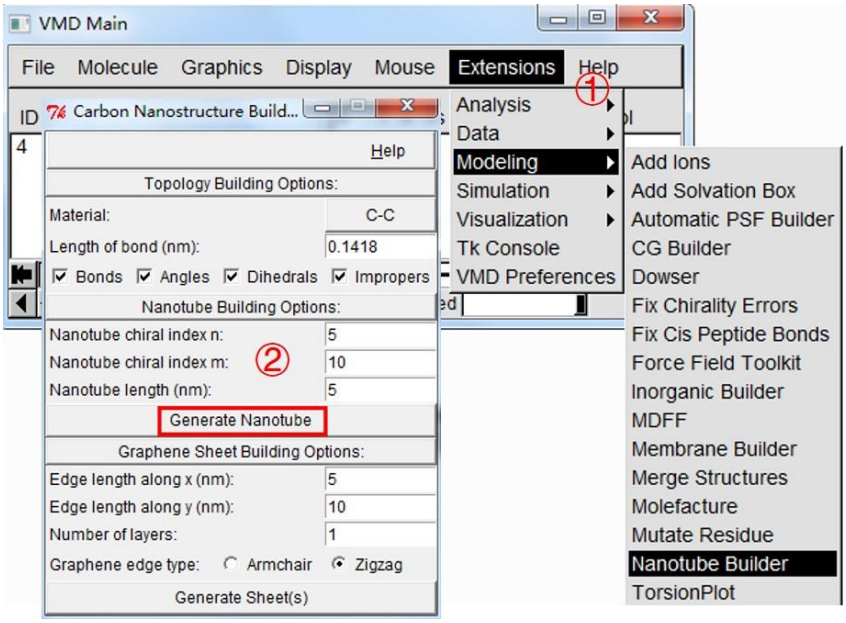

Figure 1. Building nanotube

2) Selecting any point within the built nanotube. In this tutorial, it is -0.2015 0.4185 30.147. Open the "parameter.dat" in folder "005-radiiCal\nanotube" and add this point coordinates to "cpoint". Besides, the parameter "vector" should be set as below:

---

vector 0.00 0.00 1.00

The "0.00 0.00 1.00" means radii measurement along Z-axis. "0.00 1.00 0.00" means radii

measurement along Y-axis. “1.00 0.00 0.00” means radii measurement along X-axis. The channel should be placed along any axis roughly.

3) Running command for radii calculation as below:

#> molaical.exe -channel radii -cpp parameter.dat

It will generate “channel_radii.dat”, “dot.vmd_plot” and “surf.vmd_plot”. The files of “dot.vmd_plot” and “surf.vmd_plot” can show the channel surface in VMD software. Open VMD tkConsole: Extensions→Tk Console. Then run command as below:

#> source surf.vmd_plot

You will see the dot surface of channel as in Figure 2:

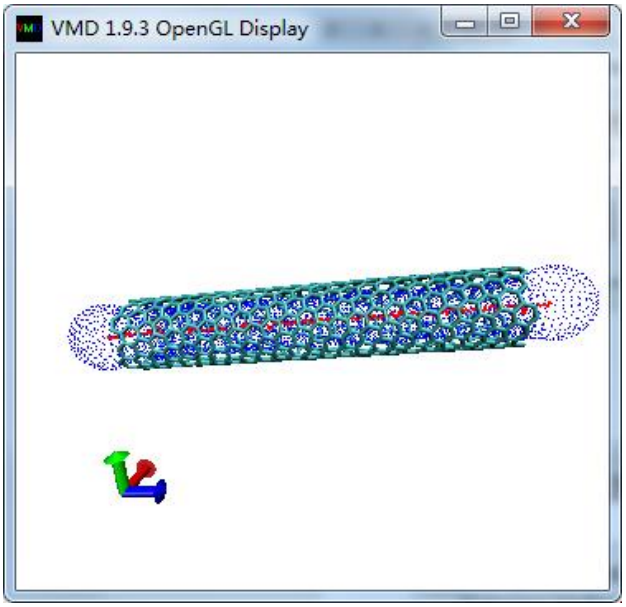

Figure 2. Surface channel of nanotube

The file of “channel_radii.dat” contains the radii values. You can plot it with OriginLab, Microsoft Excel, etc. The plotted result is shown in Figure 3:

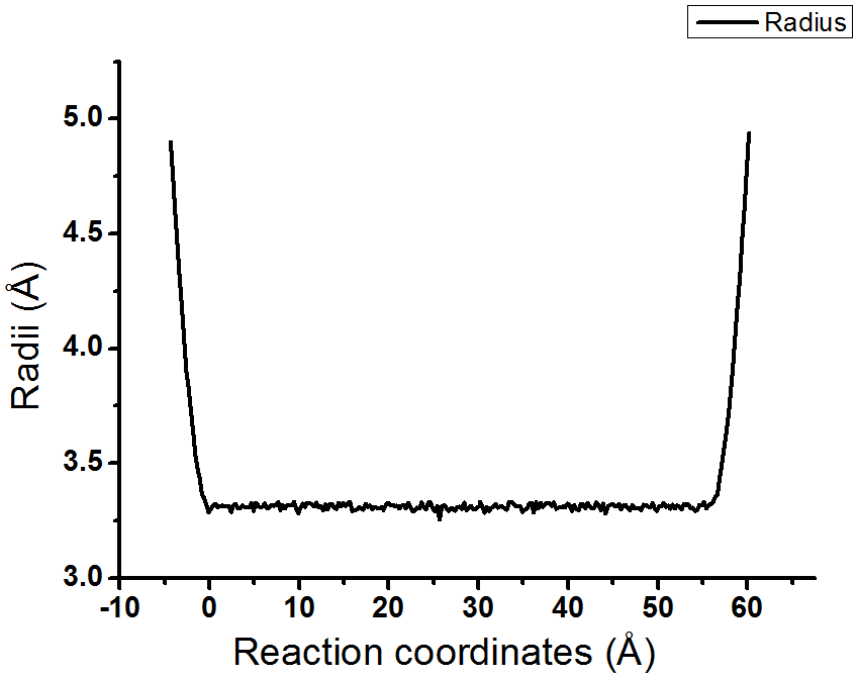

Figure 3. Radii versus reaction coordinates

3.2. Protein radii calculation

Go to the tutorial directory:

#> cd 005-radiiCal/KcsA

Selecting any point within the protein channel. The parameter "cpoint" is set to the coordinates of the selected point. The parameters "cpoint" and "vector" should be set as below:

---

cpoint 0.001 0.006 1.927

vector 0.00 0.00 1.00

The "0.00 0.00 1.00" means radii measurement along Z-axis. "0.00 1.00 0.00" means radii measurement along Y-axis. "1.00 0.00 0.00" means radii measurement along X-axis. The channel should be placed along any axis roughly.

1). Running command for radii calculation as below:

#> molaical.exe -channel radii -cpp parameter.dat

It also generates "channel_radii.dat", "dot.vmd_plot" and "surf.vmd_plot".

Open VMD tkConsole: Extensions→Tk Console. Then run command as below:

#> source surf.vmd_plot

You will see the dot surface in Figure 4:

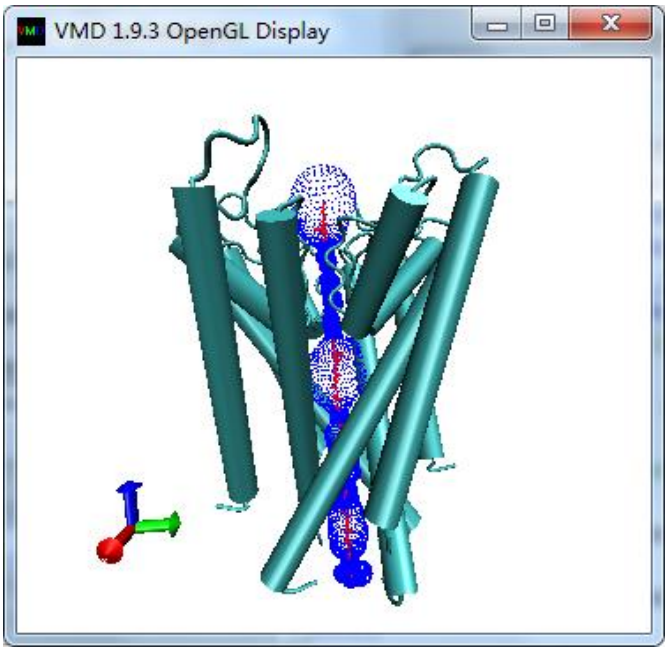

Figure 4. Dot surface in protein channel

Radii are plotted as below (see Figure 5):

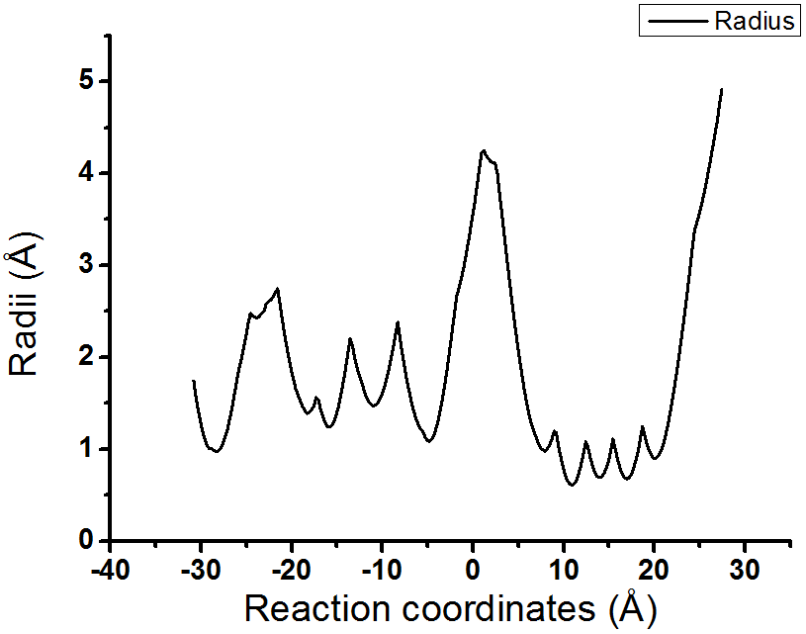

Figure 5. Radii versus reaction coordinates

Notice: the parameter "conpar" in the file "parameter.dat" is a control constant whose default value is 0.15. The high value of control constant "conpar" will increase the random measurement process. So you will find some weird paths of radii measurement at times. If the pore is very regular and along one direction of X, Y and Z axis generally, you can decrease the value of control constant "conpar" such as 0.04. But the "conpar" cannot be set to 0. In the circumstances, you will get the regular measurement path along the channel.

3.3. Advance radii calculation

This part example calculates radii of protein by PDB and PSF files which are generated by the CHARMM force field. Go to the tutorial directory:

#> cd 005-radiiCal/GramicidinA

Selecting any point within the peptide hole. The parameter "cpoint" is set to the coordinates of the selected point. The parameters "psfpath", "cpoint" and "vector" should be set as below:

---

psfpath 1JNO.psf
cpoint 0.1625 -0.629 -1.838
vector 0.00 0.00 1.00

The "0.00 0.00 1.00" means radii measurement along Z-axis. "0.00 1.00 0.00" means radii measurement along Y-axis. "1.00 0.00 0.00" means radii measurement along X-axis. The channel should be placed along any axis roughly.

1). Running command for radii calculation as below:

#> molaical.exe -channel radii -cpp parameter.dat -fc charmm

It also generates "channel_radii.dat", "dot.vmd_plot" and "surf.vmd_plot".

Open VMD tkConsole: Extensions→Tk Console. Then run command as below:

#> source surf.vmd_plot

You will see the surface in the peptide channel (see Figure 6):

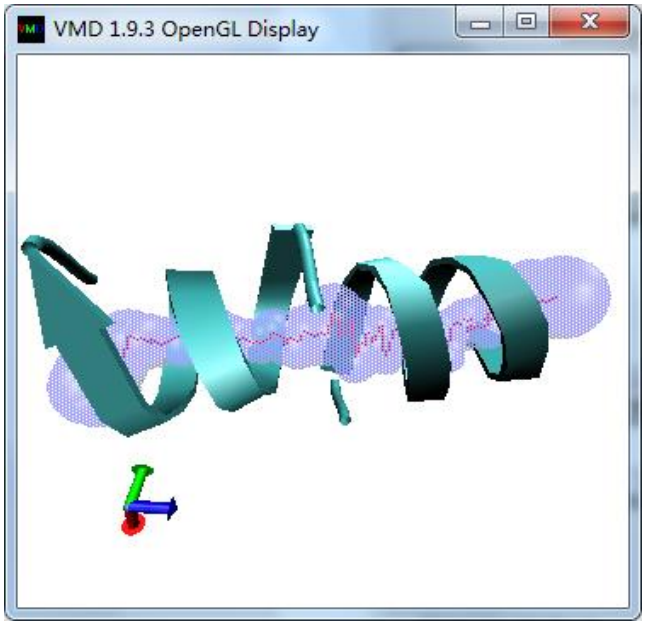

Figure 6. Dot surface in peptide channel

Radii are plotted as below (see Figure 7):

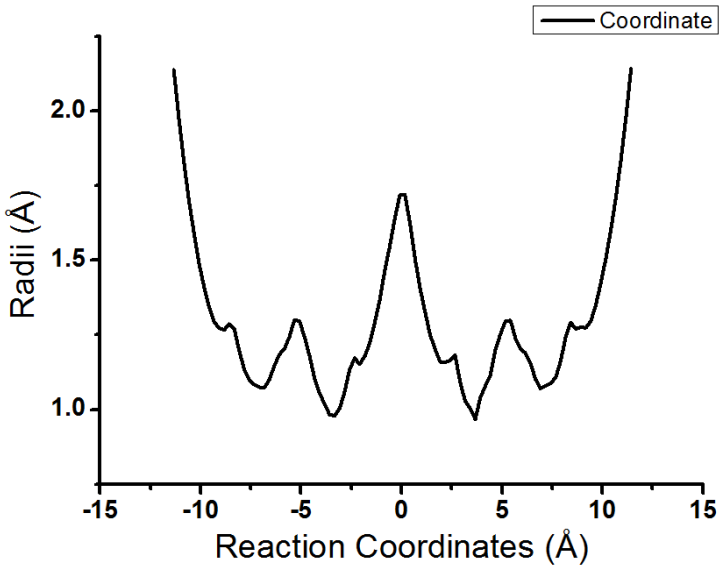

Figure 7. Radii versus reaction coordinates