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. Here, MolAICal (https://doi.org/10.1093/bib/bbaa161) is employed for this tutorial.

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).
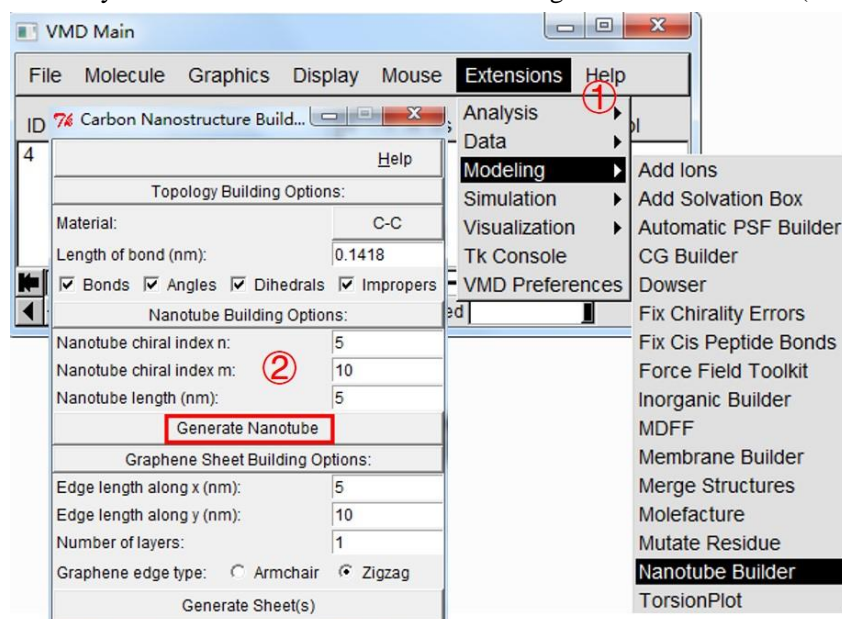
Figure 1. Building nanotube

2) Using a similar way in the window of VMD, open Tk Console: Extensions→Tk Console. Change to the directory that contains material files such as "nanotube.pdb" and "parameter.dat" by command "cd <your directory path>" in Tk Console. For example:

#> cd d:/005-radiiCal/nanotube

3) Saving the nanotube as "nanotube.pdb" by below command in Tk Console:

#> set all [atomselect top all]

#> $all writepdb nanotube.pdb

4) Selecting any point within the built nanotube. You can choose the center coordinates between two different atoms that locate at the channel surface. 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". The parameter "cpoint" and "vector" should be set as below:

----

cpoint   -0.2015 0.4185 30.147

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.

5) Running command for radii calculation in Windows DOS or Linux console 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 Tk Console using a similar way of Figure 1: Extensions→Tk Console. Then run command as below:

#> source dot.vmd_plot

We omit the way for representation of nanotube in VMD. You can set it according to your preference. You will see the dot surface of channel as in Figure 2:
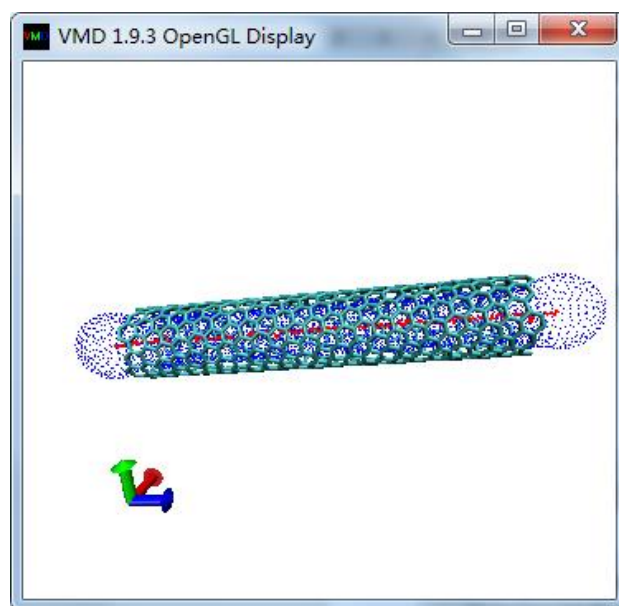
Figure 2. The channel surface of nanotube

The file of "channel_radii.dat" contains the reaction coordinates and radii values. The 1st column of "channel_radii.dat" contains reaction coordinates. The 2ed column of "channel_radii.dat" contains radii values. You can plot it with OriginLab, Microsoft Excel, etc. The plotted result is shown in Figure 3:
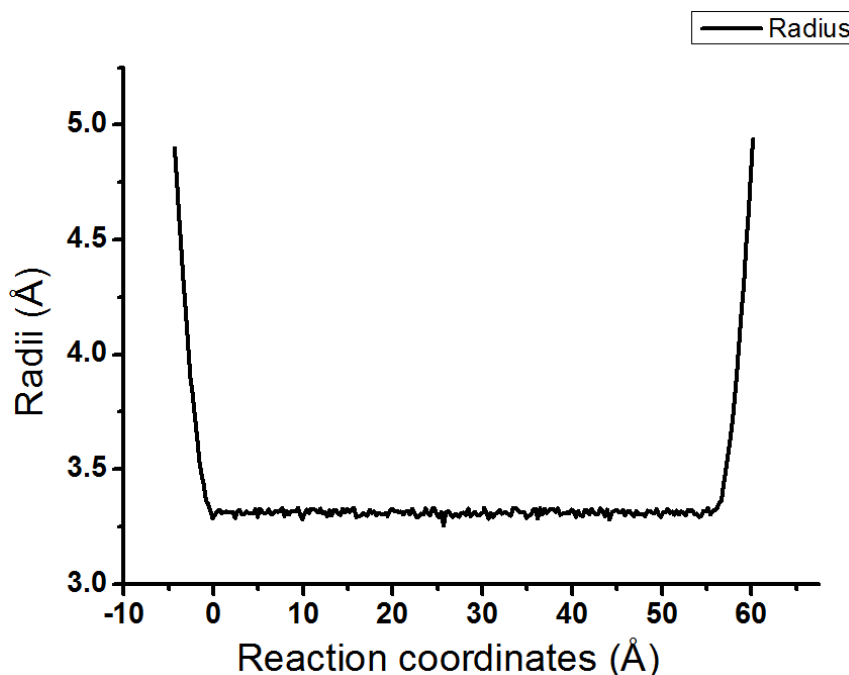
Figure 3. Radii versus reaction coordinates

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 in Windows DOS or Linux console as below:
#> molaical.exe -channel radii -cpp parameter.dat

2) It also generates "channel_radii.dat", "dot.vmd_plot" and "surf.vmd_plot". Open VMD Tk Console using a similar way of Figure 1: Extensions➔Tk Console. Then run command in Tk Console as below:
#> mol load pdb KcsA.pdb

We omit the way for representation of protein in VMD. You can set it according to your preference. You will see the dot surface in Figure 4:
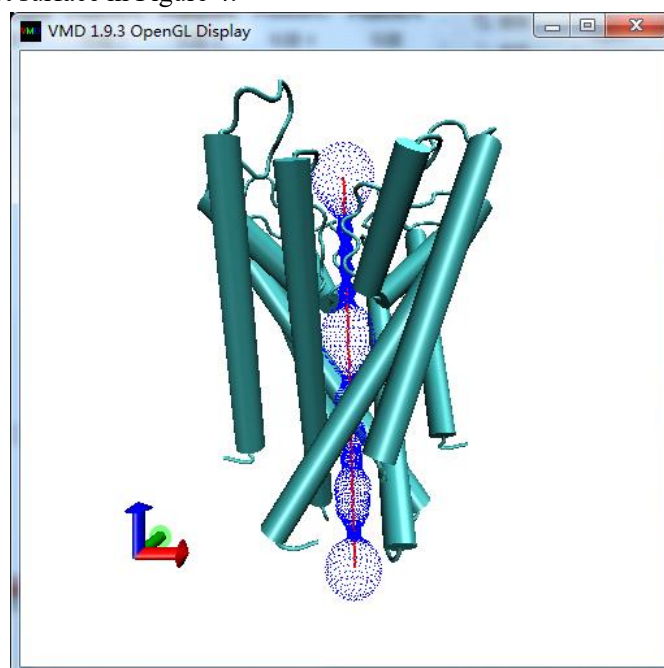
Figure 4. Dot surface in protein channel

The file of "channel_radii.dat" contains the reaction coordinates and radii values. The 1st column of "channel_radii.dat" contains reaction coordinates. The 2ed column of "channel_radii.dat" contains radii values. You can plot it with OriginLab, Microsoft Excel, etc. Radii are plotted as below (see Figure 5):
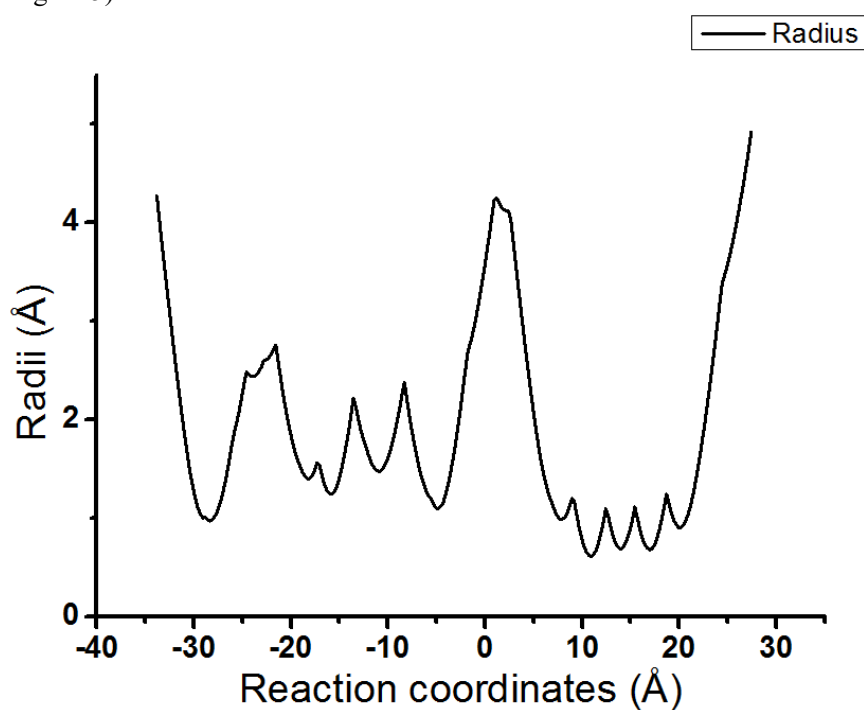
Figure 5. Radii versus reaction coordinates

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 peptide channel 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 "pdbpath", "psfpath", "cpoint" and "vector" should be set as below:

```
----------------------------------------------------------------
pdbpath        1JNO.pdb
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 in Windows DOS or Linux console as below:

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

2) It also generates "channel_radii.dat", "dot.vmd_plot" and "surf.vmd_plot". Open VMD Tk Console using a similar way of Figure 1: Extensions→Tk Console. Then run command in Tk Console as below:

#> mol load pdb 1JNO.pdb
#> source surf.vmd_plot

We omit the way for representation of peptide in VMD. You can set it according to your preference. You will see the surface in the peptide channel (see Figure 6):
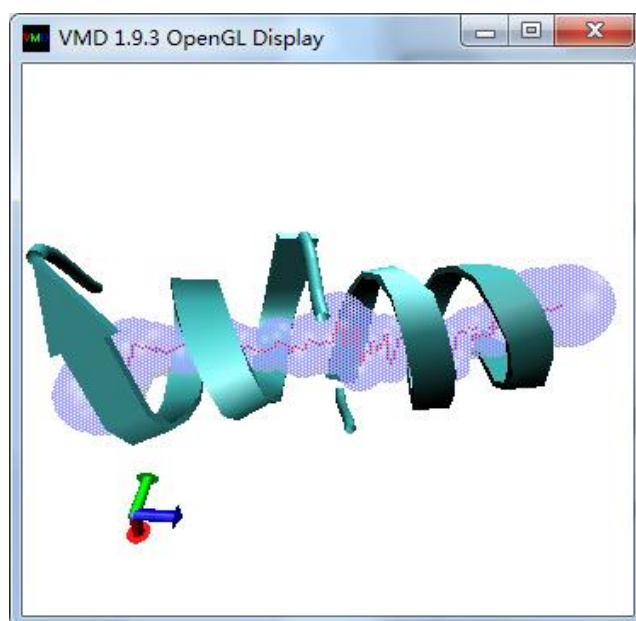
Figure 6. Dot surface in peptide channel

The file of "channel_radii.dat" contains the reaction coordinates and radii values. The 1st column of "channel_radii.dat" contains reaction coordinates. The 2ed column of "channel_radii.dat" contains radii values. You can plot it with OriginLab, Microsoft Excel, etc. Radii are plotted as below (see Figure 7):
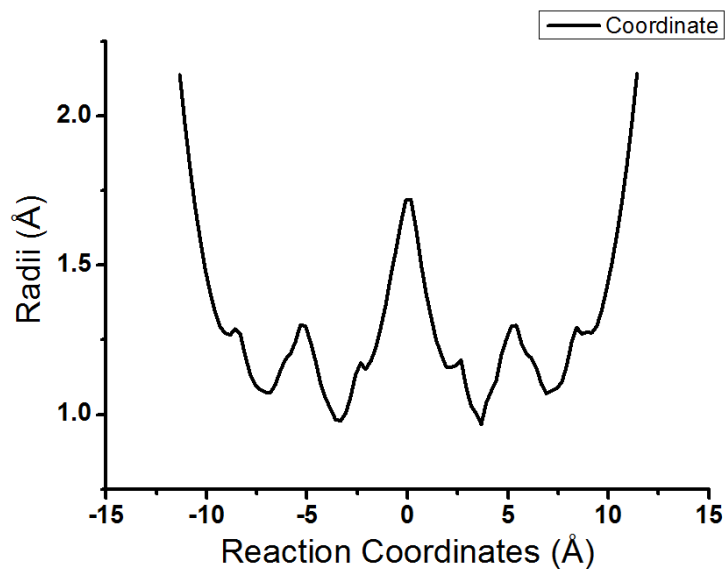
Figure 7. Radii versus reaction coordinates