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. The advance radii calculation is based on the PDB and PSF files which are produced by 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).

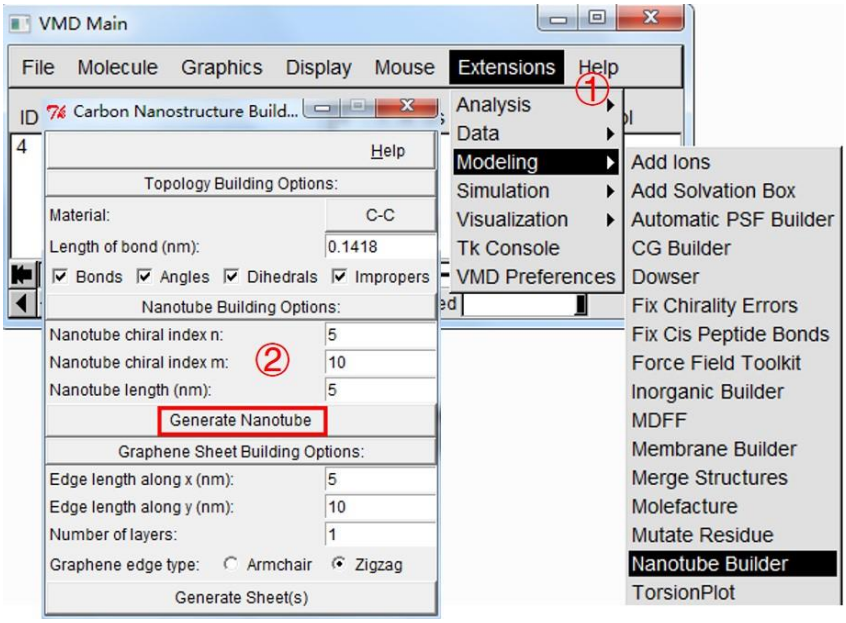


Figure 1. Building nanotube

2) Selecting a point in 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".

3) Running command for radii calculation as below:

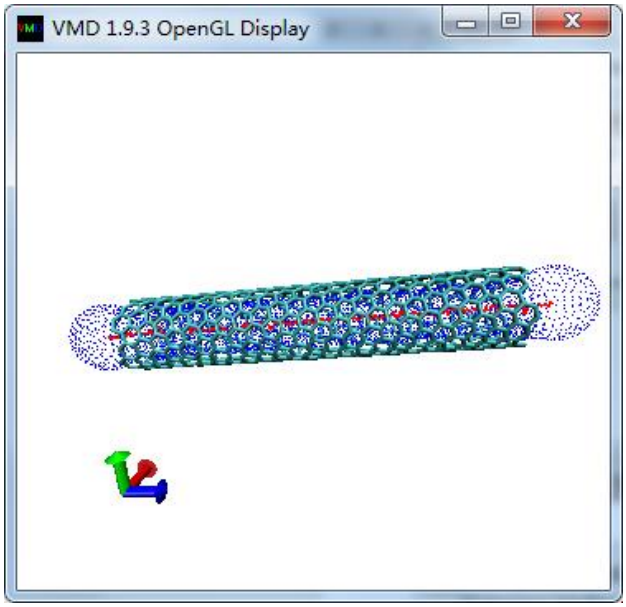
```
#> molaical.exe -channel radii -cpp parameter.dat
```

It will generate "channel_radii.dat", "dot.vmd_plot" and "surf.vmd_plot". The files of

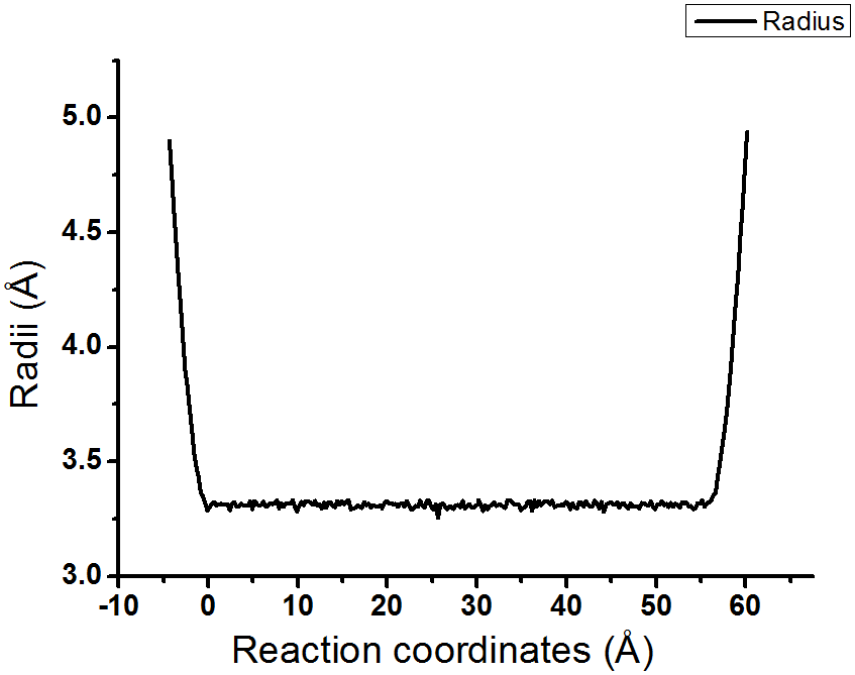
“dot.vmd_plot” and “surf.vmd_plot” can show the channel surface in VMD software. Open VMD tkConsole: Extensions→Tk Console. Then run command as below:

#> source surf.vmd_plot

You will see the below figure:



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



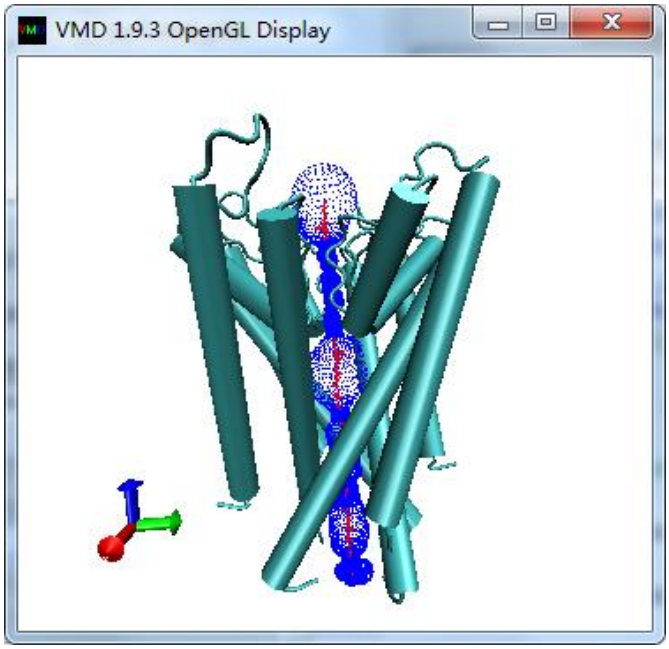
3.2. Protein radii calculation

Go to the tutorial directory:
#> cd 005-radiiCal/KcsA

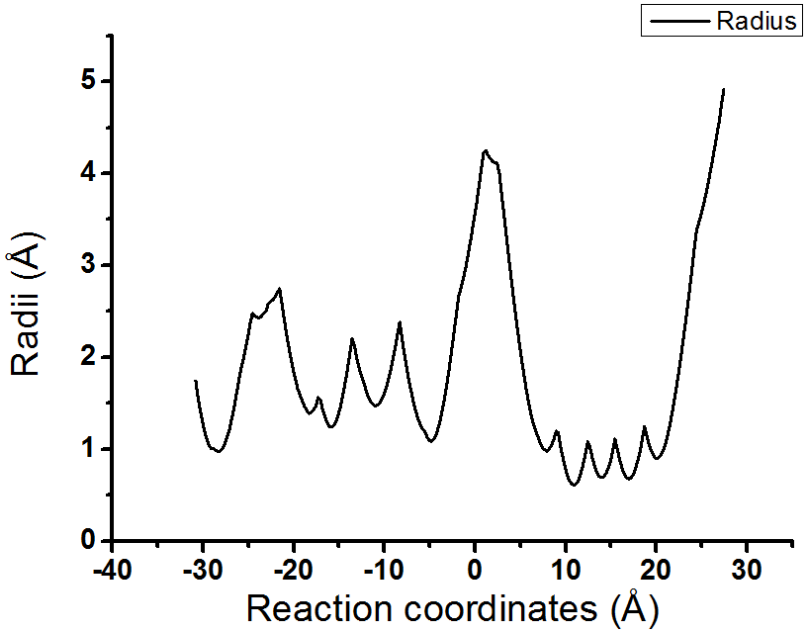
1). Running command for radii calculation as below:
#> molaical.exe -channel radii -cpp parameter.dat

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 below figure:



Radii are plotted as below:



3.3. Advance radii calculation

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

#> cd 005-radiiCal/GramicidinA

1). Running command for radii calculation as below:

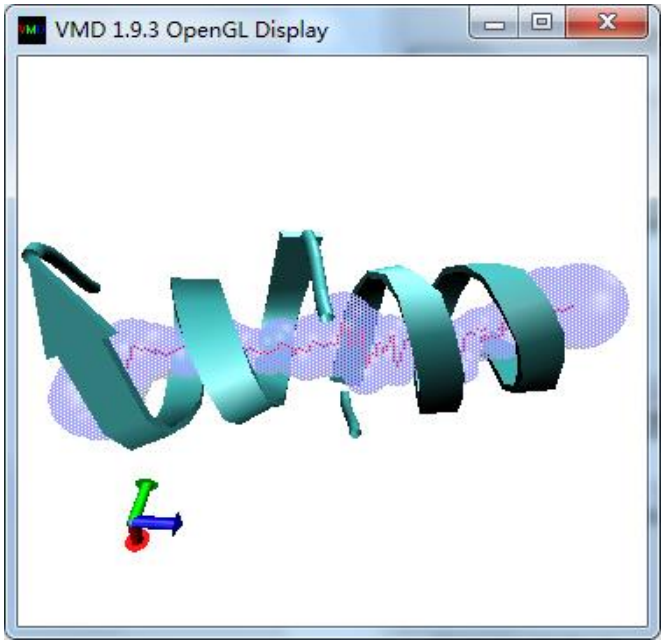
#> molaical.exe -channel radii -cpp parameter.dat -fc charmm

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 below figure:



Radii are plotted as below: