

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, peptide, protein radii calculation and advance radii calculation. 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).

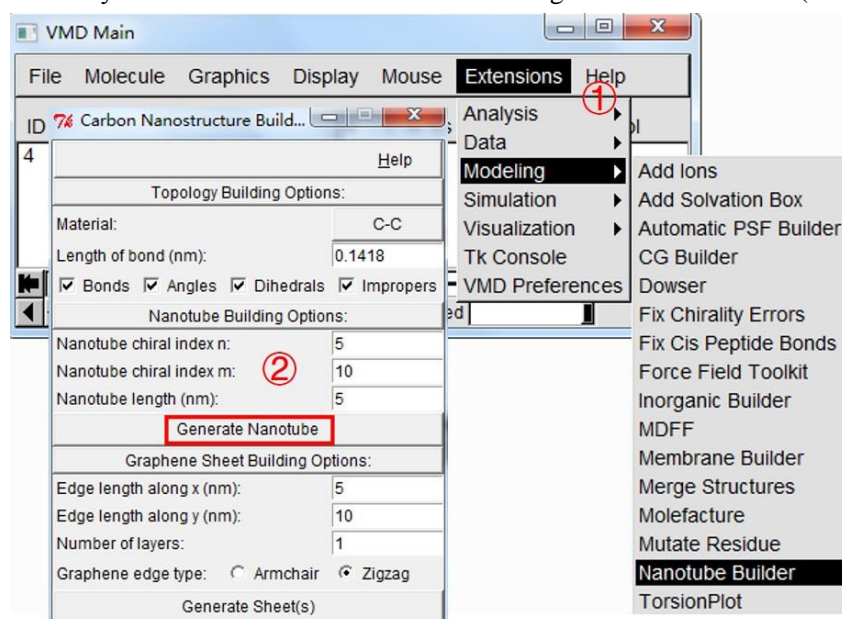


Figure 1. Building nanotube

- 2) Selecting 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”. 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:

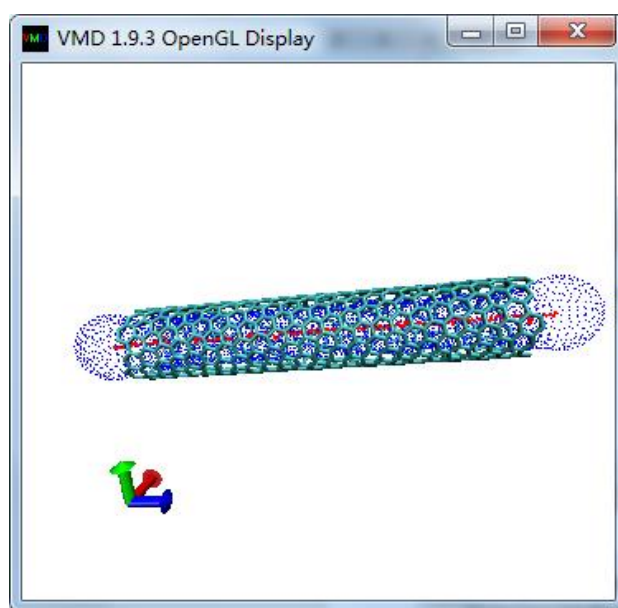


Figure 2. Surface channel of nanotube

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:

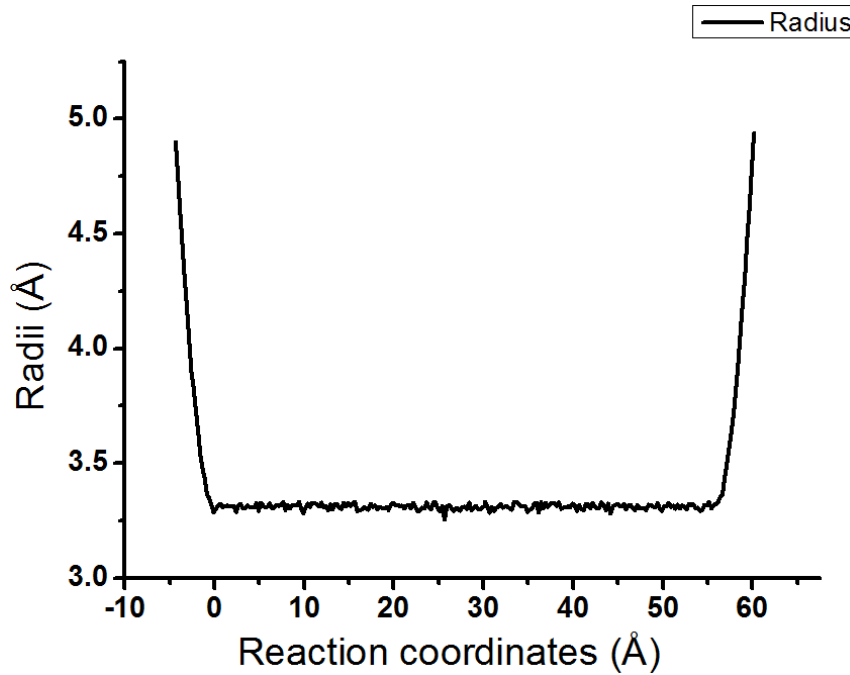


Figure 3. Radii versus reaction coordinates

3.2. Protein radii calculation

Go to the tutorial directory:

```
#> cd 005-radiiCal/KcsA
```

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:

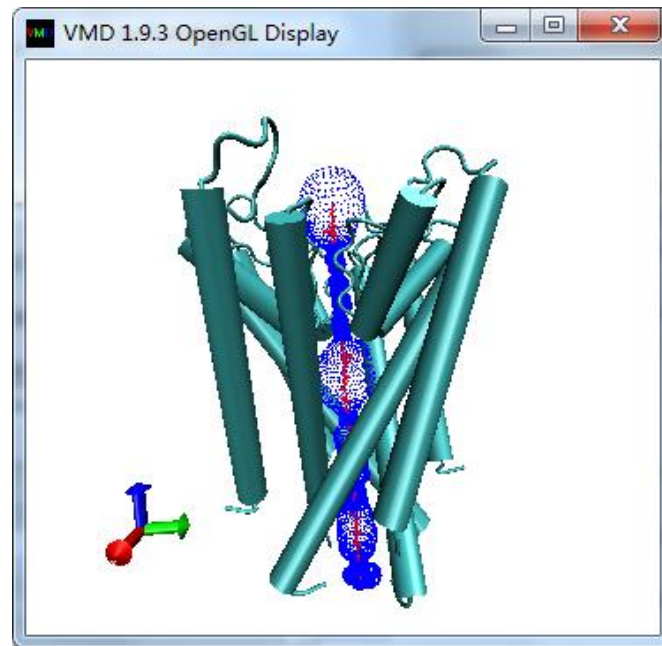


Figure 4. Dot surface in protein channel

Radii are plotted as below (see Figure 5):

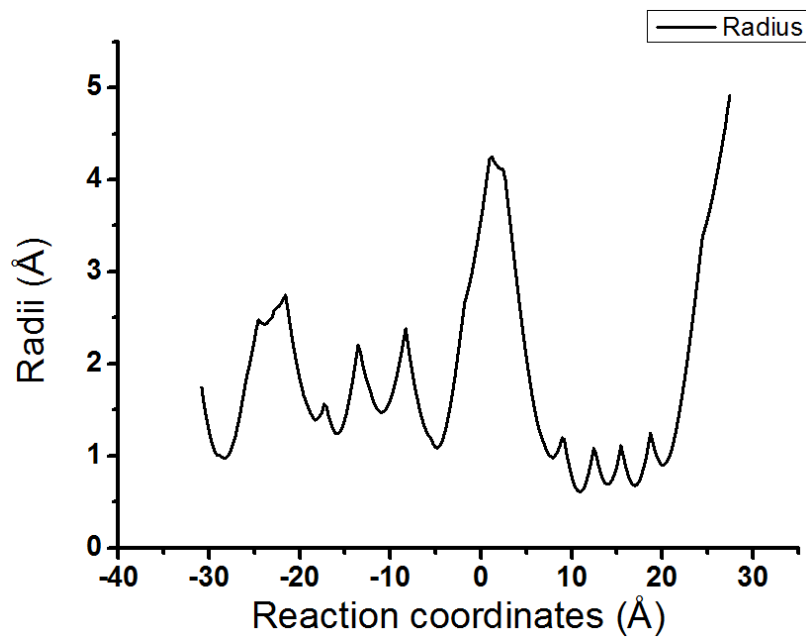


Figure 5. Radii versus reaction coordinates

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`

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):

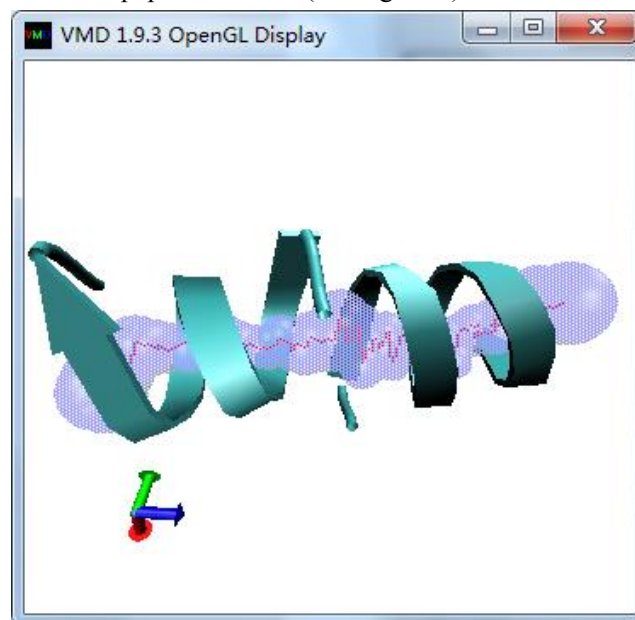


Figure 6. Dot surface in peptide channel

Radii are plotted as below (see Figure 7):

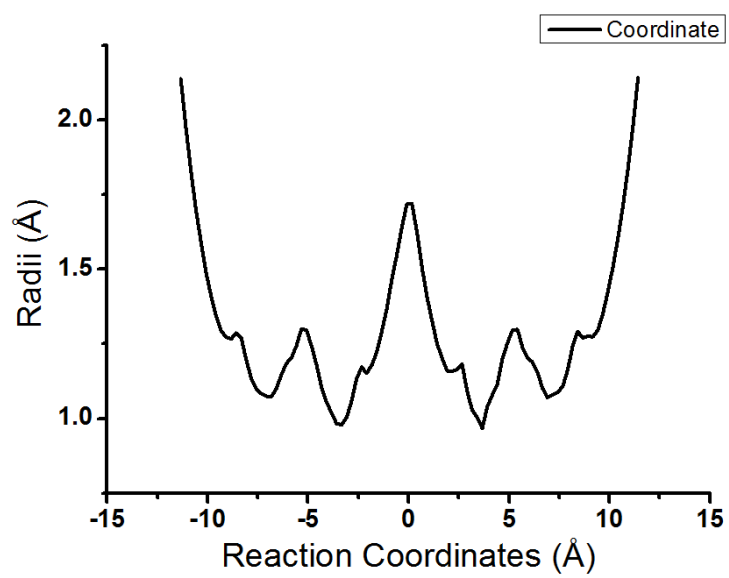


Figure 7. Radii versus reaction coordinates