# ********** DensityCalculator **********

## NOTE

Due to the size limit, the *all.dcd* file cannot be uploaded to github, please go to the article link for it,

https://www.sciencedirect.com/science/article/pii/S0010465521001442

or CPC Library link to program files,

https://doi.org/10.17632/vcbh2gt8wg.1

## File descriptions

The "***source code and examples***" folder contains 7 files, they are:

1. *dc.tcl*, the source code file;
2. *all.psf, the psf* trajectory file for examples
3. *all.dcd*, the *dcd* trajectory file for examples
4. *mass_y_0_0 (yr=232 dy=0.5).dat*, the data file generated by the code for the 1D examples
5. *mass_y_0_0 (yr=58 dy=2).dat*, the data file generated by the code for the 1D examples
6. *mass_xy_59_59_0.000_72.000 (not water).dat*, the data file generated by the code for the 2D examples
7. *mass_xy_59_59_0.000_72.000 (water)*, the data file generated by the code for the 2D examples

Note: only source code *dc.tcl* is the necessary file, the other six files are just for demonstration of the code usage.

## Installation

There are two suggested ways to install:

1. Copy *dc.tcl* to a user's directory, taking *C:/CODES* in Windows OS as example. Then add the following line of command to the file *vmd.rc* which should be located at the VMD installation folder, e.g. *C:\Program Files (x86)\University of Illinois\VMD*. Then, done.

   *source C:/CODES/dc.tcl*

2. Or, simply copy *dc.tcl* to the working directory of VMD.

In the first approach, *dc.tcl* is automatically loaded upon starting VMD; in the second approach, users need to type "*source dc.tcl*" each time when starting VMD or after modifying *dc.tcl*.

## Execution

1. On *VMD main* menu, load *Tk Console* via *Extensions→Tk Console.*
2. Proceed to the working directory by typing "*cd xxxxxx (file directory)*" in the command line interface of *Tk console*.
3. Type "*source dc.tcl*" in the command line interface of Tk console to load the code if using the second method of installation; otherwise, skip this step.
4. Type command with parameters, as described in *Usage examples* below.

## Usage examples

1D case in Fig.3:

1. Load *Tk Console* via *Extensions→Tk Console,* then proceed to the VMD working directory.
2. Put source code file *dc.tcl* and trajectory files *all.psf* and *all.dcd* into the VMD working directory.
3. Type the following command in command line interface of *Tk console*:

*dc all.psf all.dcd mass_y 0 0 1 45 85 1 0 116 232 0 72 1 {all}*

4. When the calculation completes, a data file named "*mass_y_0_0.dat*" appears in the working directory, rename it with "*mass_y_0_0 (yr=232 dy=0.5).dat*".
5. Remove the first three lines and the last line from the data file, retaining only the two columns of numbers. Use this data file to plot the 1D density profile by using a plotting software, a figure like Fig.3a can be generated.
6. Then, type the following commands, to generate another data file "*mass_y_0_0.dat*", and rename it with "*mass_y_0_0 (yr=58 dy=2).dat*". Remove the unnecessary lines and plot a figure such as Fig.3b.

*dc all.psf all.dcd mass_y 0 0 1 45 85 1 0 116  58 0 72 1 {all}*

2D case in Fig.4:

1. Type the following command to get a data file "*mass_xy_59_59_0.000_72.000*", rename it with " *mass_xy_59_59_0.000_72.000 (not water).dat*".

*dc all.psf all.dcd mass_xy 59 59 1 0 130 65 0 116 58 0 72 1 {not water}*

2. In the data file, all X Y Z position values are given, the Z position values should be removed to plot the 2D density heatmap, the final figure should look like Fig.4a (detailed colors may differ due to different plotting software and settings).
3. Type the following command to get a data file "*mass_xy_59_59_0.000_72.000*", rename it with "*mass_xy_59_59_0.000_72.000 (water).dat*".

*dc all.psf all.dcd mass_xy 59 59 1 0 130 65 0 116 58 0 72 1 {water}*

4. Take same procedures to plot a figure like Fig.4b.