LAB 3A (II): SIMULATION OF WATER PERMEATION THROUGH NANOTUBES

The goal of this lab is to learn the basics of VMD and NAMD software and to get practice with force field simulations.

Lab Procedure:

The lab is performed in VMD which you can either run through an X11-supporting terminal or on your local computer. The lab procedure *assumes independent work* with VMD and NAMD manuals. Refer to their websites for general information about running VMD and NAMD.

The NAMD manual website:
http://www.ks.uiuc.edu/Research/namd/2.10/ug/

VMD's help website:
http://www.ks.uiuc.edu/Research/vmd/vmd_help.html

Scholar's User Guide:
https://www.rcac.purdue.edu/compute/scholar/guide/

IMPORTANT: There are a few things you need to know before proceeding:

We will be using `.tar.gz` files, which is a special type of compression format. In order to *unzip* them, you will need to give two commands:

To unzip a `.tar.gz` file: `gzip -d <filename>.tar.gz`
Then do: `tar -xf <filename>.tar`

If you are running on Scholar, you will need to load the NAMD module to run NAMD simulations. *Before* running VMD, load the NAMD module with this command:

To load the NAMD module: `module load namd`

VMD is installed on iTaP computers, In case you need to install it on your computer, you may obtain a VMD installer from here:
http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD

You can also run the simulations on your local computer, using a local version of NAMD. This is not available in the iTaP computers.

If have installed VMD and are running locally, you may also want to install NAMD from here:
http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD

Step 1:

Follow the instructions of the VMD tutorial "Simulation of Water Permeation through Nanotubes" from this website:
http://www.ks.uiuc.edu/Training/Tutorials/

You may find it in the Bionanotechnology section.

Step 2: YOUR TURN

For the lab report, answer all questions along the tutorial and do the exercises.