How to install VMD and NAMD

Please go to the address http://www.ks.uiuc.edu/ and in the blue ribbon on top of the web page, you will find the Software tab in which you can hover over both VMD and NAMD separately. Click download for both or Ctrl+Click on the hyperlinks provided below. You will be required to register before download becomes available.

For Windows:

NAMD □ Win64

VMD 2 VMD 1.9.4a51 for Windows, 64-bit Intel x86 (x86 64)

For Mac:

NAMD | MacOSX-x86 64

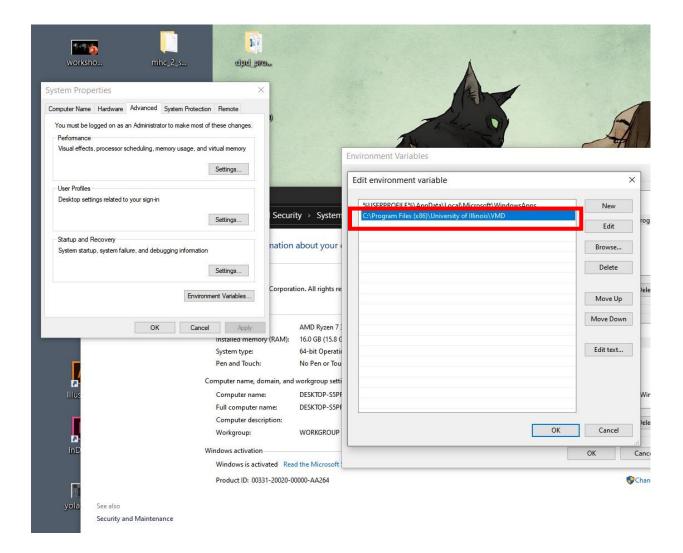
VMD □ **VMD 1.9.4a57 for MacOS X, 64-bit Intel x86 (x86 64)**

After downloading VMD and NAMD package to your computer, unzip them and put the files to a directory on your computer (Please make sure your directory does not contain any special/Turkish letters and blanks, example of a directory: C:\Users\melikeberksoz\Desktop\MIDST which means my VMD and NAMD files are in a folder named MIDST on my desktop). For Mac, simply drag both folders to your 'Applications'.

To execute software from any "working directory," by writing its name to the terminal, you should add the directory of each software as "path variables."

For Windows:

In your start menu, right click on This PC>Properties>Advanced system settings>Advanced>Environment Variables then add the directory paths of VMD and NAMD to "Path" under your user variables. Please see the figure below as an example of adding VMD to "path" in Windows 10.



For Mac:

• Start up Terminal in your home directory. Type "ls -al" to view all the files on your home directory. If a file named ".bash_profile" doesn't exist, type touch .bash_profile to create it. If it does exist or you just created one, type nano .bash_profile to open it. Once you open it, copy the following path in two separate lines:

For NAMD:

For VMD:

```
alias vmd='/Applications/VMD\ 1.9.4a57-x86_64-Rev12.app/Contents/MacOS/startup.command'
!!! Don't remove the gap in VMD path, copy it as it is !!!
```

Type ctrl+x and then Y to save it.

• If you are using .zsh instead of .bash: Open the terminal and type touch .zshrc to create a file named 'zshrc'. Then type nano .zshrc to open it. Again copy the paths given above, save and exit.

Close all terminal windows, open a new one and type **vmd** and enter to test if it is working. Do the same for **namd**.

If MacOS gives a warning about opening VMD (being an unidentified developer), go to Settings
 → Security&Privacy → General, click 'Open anyway'.

Text Editor

In this workshop, you will need a text editor which will be needed to write and edit scripts which will determine the parameters for our simulations. We recommend Visual Studio Code or Notepad++ however you are free to use a text editor such as Wordpad or any editor of your choosing if you are already familiar with another one.