MIDST GUIDE

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1. 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.

1.1 For Windows User

NAMD : Win64
VMD : VMD 1.9.4a51 for Windows, 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. Here is an example directory:
C:\Users\melikeberksoz\Desktop\MIDST
which means both VMD and NAMD files are in a folder named MIDST on my desktop)

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**."

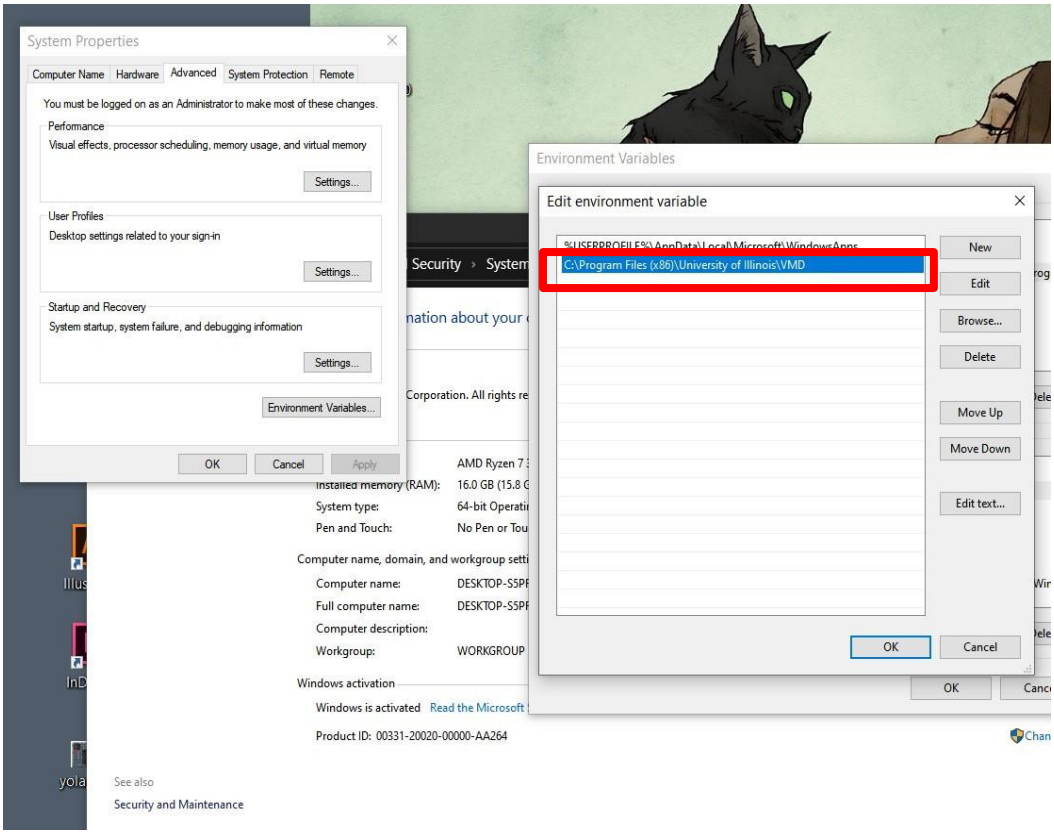
1. In your start menu, right click on:

   PC → Properties → Advanced system settings → Advanced → Environment

   Variables

2. 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.



1.2 For Mac User

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 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**."

Start up Terminal in your home directory. Type "ls -al" to view all the files on your home directory.

If a file named '.zshrc' does not exist, type `touch .zshrc` to create a file named '.zshrc'. Then type `nano .zshrc` to open it. Once you open it, copy the following path in two separate lines:

For NAMD:

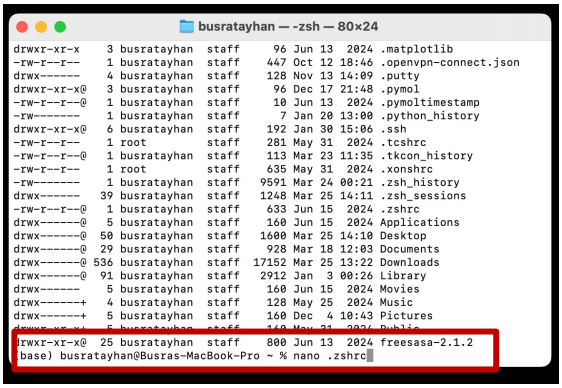
```
export  PATH=$PATH:/Applications/NAMD_2.14_MacOSX-x86_64-multicore
```

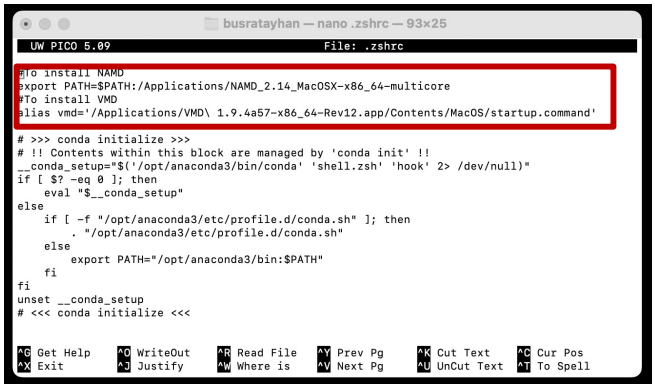
For VMD:

```
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 !!!

Please see the figure below as an example of adding VMD to "path" on Mac.





Close all terminal windows, open a new one and type **vmd** and enter to test if it is working. Do the same for **namd2**.

- If MacOS gives a warning about opening VMD (being an unidentified developer), go to:

  Settings → Security&Privacy → General , click 'Open anyway'.

2. HOW TO INSTALL CONDA & JUPYTER LAB

The installation instructions for Conda are obtained from "anaconda.installation" . This web page also provides instructional videos. It can be visited, or the installation instructions for Windows and macOS can be followed below.

2.1 For Windows User

- Download the installer from the Anaconda website **anaconda.com/download**
    - Please go to the website, enter your email, agree to the permissions, and click the Submit button.
    - From **Anaconda Installers** section, select the appropriate installer under the Windows tab
- Go to your Downloads folder and double-click the installer to launch.
- Click **Next** and then agree to the **Anaconda's Terms of Service (TOS)**.
- Select an installation option:
    - **Just Me** (Recommended): Install Anaconda Distribution for the current user account.
- Click **Next**.
- Select a destination folder to install Anaconda, then click **Next**.
- Click **Install**. Customize your installation options

2.2 For Mac & Linux User

- On anaconda.com/download, register with Anaconda (if desired), and click **Download for Mac**.
- Double-click the downloaded file and click **Continue** to start the installation.
- View the Read Me instructions and click **Continue**.
- Read through the Anaconda's Terms of Service (TOS) and click **Continue**, then click **Agree** to agree to the terms.
- Choose an install location and click **Install**

3. HOW TO INSTALL PRODY

Because ProDy requires a lower Python version (Python 3.8), it is recommended to create a Conda environment and install ProDy into this environment.

Here is how to create a Conda environment from terminal:

```
conda
conda create --name prody_env
conda activate prody_env
conda install python=3.8
```

Here is how to install ProDy into this environment:

- **If pip is installed**, run the following command

```
pip install -U ProDy
```

- **Alternatively, you can use:**

```
Conda install ProDy
```

4. HOW TO ACCESS TO TRUBA

The official TRUBA connection guide can be followed, or alternatively, the instructions provided below may be used

4.1 OpenVPN connection

For off-campus access, OpenVPN must be installed prior to connecting. This link provides details and OpenVPN files for different operating systems.

4.2 Connecting with SSH

SFTP can be used for file transfer using (SSH File Transfer Protocol):

These SFTP clients can be downloaded :

- **Cyberduck** (Mac)
- **MobaXterm** or **WinSCP** (Windows)
- **FileZilla** (cross-platform)

Once connected to the HPC system, you can drag and drop the required input files to/from the HPC directory. As the job runs, output files will appear in the same directory.

If you are connecting from the campus, that is, from computers connected to the ULAKNET network

Remote host: levrek.ulakbim.gov.tr

If you are connecting from off-campus, you must first connect to the TRUBA computers with OpenVPN to use MobaXterm.

Remote host: 172.16.11.1
Specify username: username (example:osari)
Port: 22

Then, you can connect to the TRUBA main server by typing the following command in the terminal:

```
ssh username@172.16.7.1
```

or

```
ssh username@levrek1.ulakbim.gov.tr
```

!!! Replace username with your actual TRUBA username.
Here you can see the disk quotas and computation times allocated to your account as shown below:

```
############################ USAGE ############################
  Core-Hour Usage :eurocc24  170922 / 420000 hours
  Disk Quota      :eurocc24  2311 GB / 4194 GB
  File Number Quota(%)   :eurocc24  0
  Core-Hour Usage :proj26  1.43636e+06 / 1513440 hours
  Disk Quota      :proj26  3371 GB / 7444 GB
  File Number Quota(%)   :proj26  0
  Core-Hour Usage :btayhan  36157.3 / 210000 hours
  Disk Quota      :btayhan  1674 GB / 2097 GB
  File Number Quota(%)   :btayhan  10
###############################################################


btayhan@barbun1:~$
```

5. JOB SUBMISSION

Send your job to ToSUn : ```sbatch sample.sh```

Send your job to Truba: ```sbatch sample.slurm```

- A step-by-step tutorial to familiarize yourself with Unix Shell : https://swcarpentry.github.io/shell-novice/

- For basic slurm commands: https://docs.truba.gov.tr/TRUBA/kullanici-el-kitabi/kaynakyoneticisi-isdongusu/basic_slurm_commands.html

- For batch run preparation: https://github.com/midstlab/md_simulation_run

- For detailed info for GPU/CPU usage @ ToSUn:

- For sample submission files https://github.com/midstlab/server_job_submission