

Preparing your Windows PC for work with NAMD and VMD projects.

Step 1. Install GnuWin32 on your PC

Obtain from <http://gnuwin32.sourceforge.net/>

Click on Packages under download or go to <http://gnuwin32.sourceforge.net/packages.html>

Download and install the following:

FileUtils
Gawk
TextUtils
Grep
Tar
Gzip

Include the path to the binaries in your system PATH. On your Windows 2000 desktop, right-click on My Computer and select Properties > Advanced > Environment Variables ...

Edit the Path variable under System variables. (Include **c:\progra~1\GnuWin32\bin** in your Path) All GnuWin32 utils and programs are installed to this directory.

For Win 98, you must edit the PATH statement in either your autoexec.bat or config.sys files.

Use Start > Run ... > cmd to open a command shell in WIN2000

Use Start > Run ... > command to open a command shell in WIN98

Step 2. Install of VMD

Use the setup program for windows that you downloaded from <http://www.ks.uiuc.edu/Research/vmd/> . Once installed include the path to the vmd executable in your system Path statement. (c:\progra~1\University of Illinois\VMD)

Step 3. Install of NAMD

Make a directory (folder) called **namd** in your c: drive.

Unzip (Untar) the binary distribution that you downloaded from <http://www.ks.uiuc.edu/Research/namd/> into c:\namd. (Do not use folder names in expanding this distribution.)

Include the path to **c:\namd** in your system path statement.

Obtain the **namdplot/namddat** scripts from <http://www.ks.uiuc.edu/Research/namd/utilities/> . These are unix shell scripts that are useful for extracting data from your namd run log file. The namdplot script will spawn a plotting program called “Grace” (<http://plasma-gate.weizmann.ac.il/Grace/>). The namdplot and namddat scripts only work from a unix platform (not linux!). If you do not have the Grace program on your unix system, use the namddat script. Namddat will output a data file that you can read into MS Excel as a space delimited file. Copy your log file and the namddat script to any unix system (e.g. rwja.umdj.edu or eden.rutgers.edu). Make the script executable then run as follows (where % is just a unix prompt):

```
% chmod 755 namddat
% ./namddat TOTAL yourjob.log
```

Will output the data (TOTAL energy in this example) to a file called *data.dat*. Rename the data.dat file

```
% mv data.dat mydata_total.dat
```

Then sftp to your Windows machine.

Step 4. Download and install ActiveState Perl for Windows.

Obtain the setup program from http://www.activestate.com/Products/Language_Distributions/ .

Step 5. Download and install ImageMagick

This software is useful for converting and manipulating image files.

Obtain the program from <http://www.imagemagick.org/> .