1 Loading Software

Reference the environment modules: http://nyuad.nyu.edu/content/dam/departments/research/hpc/hpc-enviroment-modules.pdf/

Software usually needs specific settings of environmental variables. NYUAD HPC uses an open source software package called "Environment Modules," (or Modules for short) which allows you to add various path definitions to your shell environment. Default compilers, applications and libraries can be set by individual or combinations of Modules commands. Modules are not applications; rather they simply add the location of applications to your environment. So you can load "modules" to set up the environment which is necessary for the software.

You can list the available Modules using the command module avail.

```
$ module avail
```

The content may vary on different clusters. If you would like to run the "vmd" program, for example, you need to first find "vmd" in this list (vmd/1.9.1) and type,

```
$ module load vmd/1.9.1
```

The "module load" command loads all the configuration information for the specific software.

Then you will be able to execute "vmd" by simply typing vmd.

In case the module did not load or a different module was loaded by mistake, the which command will return an error:
$ which vmd
/usr/bin/which: no vmd

![Note]

Some modules might depend on other modules.

For example, you will encounter an error message like shown below if you try to load Amber 12 directly;

```
$ module load amber/mvapich2/intel/12
amber/mvapich2/intel/12(16):ERROR:151: Module 'amber12/mvapich2/intel/12'
depends on one of the module(s) 'intel/12.1.3'
amber/mvapich2/intel/12 (16):ERROR:102: Tcl command execution failed: prereq
intel/12.1.3
```

In this case, you have to load the Intel (Intel C/C++/Fortran compiler) first.

The correct method to do so is to as follows:

```
$ module load intel/12.1.3 (as well as loading all the other prerequisite
modules)
```

THEN

```
$ module load amber/mvapich2/intel/12
```