

Current way of using programs

#####

List available programs:

 module avail

List loaded programs:

 module list

Load a program:

 module load <program>

Unload a program

 module unload <program>

Show info for program e.g. path to program

 module show <program>

example :

 \$module load atsas

 \$ module show atsas

/home/tp# module show atsas

/usr/local/modules/modulefiles/atsas/2.8.3-1:

module-whatis Setup atsas 2.8.3-1

conflict atsas

prepend-path PATH /usr/local/modules/atsas/2.8.3-1/bin

Older version notes (may be outdated)

#####

CCP4 / shelx / arp / warp :

 source /usr/local/ccp4-7.0/bin/ccp4.setup-sh

 or setccp4

XDS version 2018:

 \$module load xds

 and the XDS bin folder will be in the PATH

phenix :

 source /usr/local/phenix-1.10.1-2155/phenix_env.sh

 or setphenix

chimera version 1.12 :

 \$module load chimera

 and the CHIMERA bin folder will be in the PATH

pymol is in the PATH :

 pymol

 or (stock from packages) : /usr/bin/pymol

EMAN2.1 :

 source /usr/local/EMAN2.1/eman2.bashrc

 or seteman

EMAN1.9 :

 source /usr/local/EMAN1/eman.bashrc

 boxer is then available

coot version 0.8.7 :

```
$module load coot  
$coot  
  
relion version 2.1:  
$module load relion  
$relion
```

```
ccpnmp :  
installed in /usr/local/ccpnmr  
analysis is in the PATH
```

```
ATSAS 2.8.3-1:  
$module load atsas  
and the ATSAS bin folder will be in the PATH
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```
imagic :  
source /usr/local/imagic/bashrc  
i
```

```
3D acceleration  
- for nvidia :  
sudo apt install nvidia-361 (packages should be available in cache) then reboot
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