

This is how to compile [VMD](#) from source and is explicitly for my desktop machine, cyclops, running X86_64 Ubuntu 10.04.4 with the aim to getting [IED](#) to work correctly. The main issue here is that the version of python that ships with VMD is different to the system python and causes all kinds of issues with external python scripts.

This solves this issue by compiling VMD against the system python version. A second issue is resolved by some modifications to the ied code which were obtained from a mailing list post.

1) Obtain VMD 1.9 [source](#)

```
ad52f695bdab5b94b860f82e88ed5c18 vmd-1.9.src.tar.gz
```

2) Install the following packages

```
sudo apt-get install libglu1-mesa mesa-common-dev libgl1-mesa-dri libglu1-mesa-dev xlibmesa-g1-dev
sudo apt-get install tk8.4-dev tk-dev libfltk1.1 libfltk1.1-dev libtachyon-dev libnetcdf-dev
```

3) Extract

```
cd /home/mw529/code/VMD/d1
tar xzf vmd-1.9.src.tar.gz
```

4) Build the plugins first

```
cd plugins
export PLUGINDIR=/home/mw529/code/VMD/d1/vmd-1.9/plugins
make LINUXAMD64 TCLINC=-I/usr/include/tcl8.4/ \
      TCLLIB=-F/usr/lib/ \
      NETCDFLDFLAGS=-lnetcdf \
      NETCDFLIB=/usr/lib/libnetcdf.so \
      NETCDFINC=/usr/include
make distrib
```

5) Set the python paths correctly

```
export PYTHON_INCLUDE_DIR=/usr/include/python2.6
export PYTHON_LIBRARY_DIR=/usr/lib/python2.6/config
```

6) Ensure the TCL dir is set correctly

```
export TCL_INCLUDE_DIR=/usr/include/tcl8.4/
```

7) Configure vmd

```
cd ../vmd-1.9
./configure LINUXAMD64 OPENGL FLTK TK IMD SILENT TCL PTHREADS PYTHON NUMPY NETCDF
cd src
```

8) In the Makefile, change:

```
INCDIRS:
-I../lib/python/lib_LINUXAMD64/lib/python2.5/site-packages/numpy/core/include
to
-I../lib/python/lib_LINUXAMD64/lib/python2.6/site-packages/numpy/core/include

LIBS:
-lpython2.5 to -lpython2.6
```

9) Build it

```
make veryclean
make
```

10) Set the following environment variables

```
export PYTHONPATH=/home/mw529/code/VMD/d1/vmd-1.9/python
export VMDDIR=/home/mw529/code/VMD/d1/vmd-1.9
```

11) Run VMD

```
/home/mw529/code/VMD/d1/vmd-1.9/LINUXAMD64/vmd_LINUXAMD64
```

12) Obtain IED

```
wget http://mccammon.ucsd.edu/ied/ied-2.02.tgz
tar xfvz ied-2.02.tgz
cd ied-2.02
```

13) Obtain the modified ied from Jerome Henin and overwrite the original

```
wget http://www.ks.uiuc.edu/Research/vmd/ mailing\_list/vmd-1/att-16740/ied.py.gz
gunzip ied.py.gz
```

14) Run ied

```
menu main on
gopython /home/mw529/code/ied/ied-2.02/ied.py
```

15) Sample inputs can be found here:

```
wget http://mccammon.ucsd.edu/ied/ied-sample-data.tar.gz
```

Note, any errors pertaining to “ImportError: No module named LinearAlgebra” can be resolved by installing python-numeric-ext:

```
apt-get install python-numeric-ext
```

Refs

http://debianclusters.org/index.php/NAMD:_Building_vmd

http://www.ks.uiuc.edu/Research/vmd/mailling_list/vmd-l/17060.html

<http://wiki.python.org/moin/TkInter>

<http://www.nexenta.org/attachments/30/python2.5.txt>