

VMD-1.9.3 for LX

ウェブページ

<http://www.ks.uiuc.edu/Research/vmd/>

バージョン

1.9.3

ビルド環境

- Intel Compiler 17.0.4.196
- GNU Compiler 4.8.5

ビルドに必要なファイル

- vmd-1.9.3.src.tar.gz
- vmd-1.9.3.bin.LINUXAMD64-CUDA8-OptiX4-OSPRay111p1.opengl.tar.gz
- tachyon-0.99b6.tar.gz

ビルド手順

```
#!/bin/csh -f
umask 022
set file_vmd_source=/home/users/ms0/build/vmd193/vmd-1.9.3.src.tar.gz
set file_vmd_binary=/home/users/ms0/build/vmd193/vmd-1.9.3.bin.LINUXAMD64-CUDA8-OptiX4-OSPRay111p1.opengl.ta
set file_tachyon=/home/users/ms0/build/vmd193/tachyon-0.99b6.tar.gz
set work=/work/users/${USER}
#-----
setenv VMDINSTALLBINDIR /local/apl/lx/vmd193/bin
setenv VMDINSTALLLIBRARYDIR /local/apl/lx/vmd193/lib
setenv CPATH /usr/include/python2.7:${work}/vmd-1.9.3/lib/tachyon/src:${CPATH}
setenv TCLINC -l/usr/include
setenv TCLLIB -L/usr/lib64
setenv PLUGINDIR ${work}/vmd-1.9.3/plugins
#-----
cd ${work}
rm -rf plugins vmd-1.9.3
tar xzf ${file_vmd_source}
tar xzf ${file_vmd_binary} vmd-1.9.3/lib/surf/surf_LINUXAMD64 vmd-1.9.3/lib/stride/stride_LINUXAMD64
cd ${work}/plugins
make LINUXAMD64
make distrib
#
cd ${work}/vmd-1.9.3/lib
tar xzf ${file_tachyon}
cd ${work}/vmd-1.9.3/lib/tachyon/unix
make linux-64-thr
cd ${work}/vmd-1.9.3/lib/tachyon/compile/linux-64-thr
cp libtachyon.a ${work}/vmd-1.9.3/lib/tachyon
cp tachyon ${work}/vmd-1.9.3/lib/tachyon/tachyon_LINUXAMD64
#
cd ${work}/vmd-1.9.3
sed -i '2iunsetenv XMODIFIERS' bin/vmd.csh
sed -i '2iunset XMODIFIERS' bin/vmd.sh
sed -i 's/python2.5/python2.7/g' ./configure
sed -i 's/-ltachyon/..\\lib\\tachyon\\libtachyon.a/' ./configure
./configure LINUXAMD64 OPENGL FLTK TK LIBTACHYON NETCDF COLVARS TCL PYTHON PTHREADS NUMPY SILENT NOSTA
cd src
make -j 20
make install
```

