

Subject: Re: AtomEye question: should I compile from source?

From: "Cook, Rich" <cook47@llnl.gov>

Date: 9/12/2012 6:57 PM

To: "Cook, Rich" <cook47@llnl.gov>

CC: Ju Li <liju@mit.edu>

I got it to build on our RHEL6 cluster with a few problems.

FYI, here is my build script.

I suggest you let the user pick a fortran compiler; I had to use ifort instead of ifc.

Also, MKL was in another directory and needed -liomp5 and other stuff.

Anyhow, FWIW! 😊

Thanks

```
#!/usr/bin/env bash
```

```
errexit() {  
    echo $1  
    exit 1  
}
```

```
#rm -rf Src  
#tar -xzf Src.tar.gz  
export hosttype=linux  
# (or aix alpha CYGWIN HPUX irix64 OSF1 sun4 sgi Darwin DarwinIntel386)  
export SYS=`uname`
```

```
INSTALL_DIR=/nfs/tmp2/rcook/AtomEye/Install  
SRC_DIR=/nfs/tmp2/rcook/AtomEye/Src  
MKL_DIR=/usr/local/tools/mkl-10.1.1.019
```

```
export LIB_PATH=$INSTALL_DIR/$SYS_TYPE/Lib  
export BIN_PATH=$INSTALL_DIR/$SYS_TYPE/Bin  
export INC_PATH=$INSTALL_DIR/Include  
export MAN_PATH=$INSTALL_DIR/Man
```

```
mkdir -p $LIB_PATH $BIN_PATH $INC_PATH $MAN_PATH
```

```
for dir in Timer/ IO/ Scalar/ VecMat/ VecMat2/ VecMat3/ Min/ Atoms/ AX/ A/; do  
    pushd $SRC_DIR/$dir  
    if [ ! -f Makefile.orig ]; then  
        cp Makefile Makefile.orig  
    fi  
    sed -e 's/-axKWNBP//g' -e 's/-lguide//g' -e 's/ifc/ifort/g' -e 's:/usr/lib/:  
/usr/lib64/:g' -e 's:/opt/intel/mkl70/lib/32/${MKL_DIR}/lib:g' -e 's/-lmkl_ia32/-lmkl  
-liomp5/g' -e 's:\(\${EXESUFFIX} \${LDFLAGS}\):\1 -Wl,-rpath -Wl,${MKL_DIR}/lib:'  
Makefile.orig > Makefile  
    gmake -j || errexit "Build failed in $dir"  
    gmake install || errexit "Install failed in $dir"  
    popd  
done  
exit 0
```

On Sep 11, 2012, at 5:31 PM, Cook, Rich wrote:

Thanks!

On Sep 11, 2012, at 5:31 PM, Ju Li wrote:

Dear Rich,

Please find the source at:

<http://li.mit.edu/Archive/Co/Src/>
Src.tar.gz
readme.txt

binary libs at:

<http://li.mit.edu/Archive/Co/i686Lib/>

Thanks!

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On 09/11/2012 08:23 PM, Cook, Rich wrote:

Hi, Sorry to barge in unannounced, but I work on our supercompute clusters to support our scientists here at LLNL, and have been asked to troubleshoot an issue with AtomEye under RHEL 6 linux. When we run A.i686 on RHEL6, we see this:

```
rcook@edge83 (AtomEye): ./A.i686 36.pdb _X11TransSocketINETConnect()  
can't get address for edge83:6014: Name or service not known error:  
AX_openwindow: cannot open X display. : Invalid argument
```

But on RHEL5, A.i686 runs normally. I suspect that some system behavior under RHEL6 has changed and for some reason the wrong ethernet interface is being used for connecting to remote X servers, which is not being caught by whatever version of libX11 you compiled with. I see that A.i686 is statically linked, and was wondering if you have another binary that is more recent or have source and compile instructions to see if that fixes our problem. Any guidance is welcome and appreciated!

Thanks!

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