Amber12-bf21 for UV2000

Webpage

http://ambermd.org/

Version

Amber 12 bugfix 21 + AmberTools 13 bugfix 20

Tools for Compiling

- Intel Compiler 11.1.080
- SGI MPT 2.07

Necessary Files for Compiling

- Amber12.tar.bz2
- AmberTools13.tar.bz2
- Patches in http://ambermd.org/bugfixes12.html
- Patches in http://ambermd.org/bugfixesat.html

Procedure of Compiling

```
#!/bin/csh -f
umask 022
# Directory for installation must be the same as working directory. Otherwise, mpi4py canno
set work="/local/apl/uv/amber12-bf21"
set build="/home/users/${USER}/build/amber12"
setenv AMBERHOME "$work"
setenv DO_PARALLEL "mpirun -np 2"
# Delete old files.
if (-d $AMBERHOME) then
if (-e $AMBERHOME/configure) then
echo "Remove $AMBERHOME to be clean."
exit 1
endif
if (! -d $AMBERHOME) then
echo "Create $AMBERHOME before build."
exit 1
endif
#
cd $AMBERHOME
bunzip2 -c ${build}/Amber12.tar.bz2 | tar xf -
bunzip2 -c ${build}/AmberTools13.tar.bz2 | tar xf -
mv amber12/* .
rmdir amber12
cd $AMBERHOME
```

```
foreach i (${build}/patches/AmberTools13 ${build}/patches/Amber12)
foreach j ($i/*.? $i/*.??)
patch -p0 < $j
end
end
#
# To get compiler version correctly, set LANG environment value.
setenv LANG C
# SSE_TYPES environment value means option "-ax${SSE_TYPES}", so unset it.
unsetenv SSE_TYPES
# If you use intel compiler version 12,
#     rism1d will be aborted and test of MPI fail.
source /opt/intel/Compiler/11.1/080/bin/iccvars.csh intel64
source /opt/intel/Compiler/11.1/080/bin/ifortvars.csh intel64
#
echo "[CPU serial edition]"
./configure --no-updates intel
make -j 16 install
#make test
make clean
echo "[CPU parallel edition]"
./configure --no-updates -mpi intel
make -j 16 install
make test
make clean
```