

Amber12-bf7 for UV2000

Webpage

<http://ambermd.org/>

Version

Amber 12 bugfix 7 + AmberTools 12 bugfix 5

Tools for Compiling

- Intel Compiler 11.1.080
- SGI MPT 2.07

Necessary Files for Compiling

- Amber12.tar.bz2
- AmberTools12.tar.bz2
- Patches in <http://ambermd.org/bugfixes12.html>
- Patches in <http://ambermd.org/bugfixesat.html>

Preparation of Wrapper Commands for Compiler

Put the following wrapper commands in `/home/users/$USER/compiler/ccuv/intel-11.1`.

mpicc

```
#!/usr/bin/perl
#
use strict;
use warnings;
my @extra;
my $compiler = "/opt/sgi/mpt/mpt-2.05/bin/mpicc";
for (my $i = 0; $i < scalar(@ARGV); ++$i) {
    if ($ARGV[$i] eq "-o") {
        @extra = ("-WI,--disable-new-dtags",
                  "-WI,-rpath,/opt/intel/Compiler/11.1/080/lib/intel64",
                  "-WI,-rpath,/opt/intel/Compiler/11.1/080/mkl/lib/em64t");
    }
}
system($compiler, @extra, @ARGV);
```

mpif90

```
#!/usr/bin/perl
#
use strict;
use warnings;
my @extra;
my $compiler = "/opt/sgi/mpt/mpt-2.05/bin/mpif90";
for (my $i = 0; $i < scalar(@ARGV); ++$i) {
    if ($ARGV[$i] eq "-o") {
        @extra = ("-WI,--disable-new-dtags",
                  "-WI,-rpath,/opt/intel/Compiler/11.1/080/lib/intel64",
                  "-WI,-rpath,/opt/intel/Compiler/11.1/080/mkl/lib/em64t");
    }
}
system($compiler, @extra, @ARGV);
```

icc

```
#!/usr/bin/perl
#
use strict;
use warnings;
```

```

my @extra;
my $compiler = "/opt/intel/Compiler/11.1/080/bin/intel64/icc";
for (my $i = 0; $i < scalar(@ARGV); ++$i) {
    if ($ARGV[$i] eq "-o") {
        @extra = ("-WI,--disable-new-dtags",
            "-WI,-rpath,/opt/intel/Compiler/11.1/080/lib/intel64",
            "-WI,-rpath,/opt/intel/Compiler/11.1/080/mkl/lib/em64t");
    }
}
system($compiler, @extra, @ARGV);

```

icpc

```

#!/usr/bin/perl
#
use strict;
use warnings;
my @extra;
my $compiler = "/opt/intel/Compiler/11.1/080/bin/intel64/icpc";
for (my $i = 0; $i < scalar(@ARGV); ++$i) {
    if ($ARGV[$i] eq "-o") {
        @extra = ("-WI,--disable-new-dtags",
            "-WI,-rpath,/opt/intel/Compiler/11.1/080/lib/intel64",
            "-WI,-rpath,/opt/intel/Compiler/11.1/080/mkl/lib/em64t");
    }
}
system($compiler, @extra, @ARGV);

```

ifort

```

#!/usr/bin/perl
#
use strict;
use warnings;
my @extra;
my $compiler = "/opt/intel/Compiler/11.1/080/bin/intel64/ifort";
for (my $i = 0; $i < scalar(@ARGV); ++$i) {
    if ($ARGV[$i] eq "-o") {
        @extra = ("-WI,--disable-new-dtags",
            "-WI,-rpath,/opt/intel/Compiler/11.1/080/lib/intel64",
            "-WI,-rpath,/opt/intel/Compiler/11.1/080/mkl/lib/em64t");
    }
}
system($compiler, @extra, @ARGV);

```

Procedure of Compiling

```

#!/bin/csh -f
umask 022
# Set working directory.
set work="/week/users/${USER}"
setenv AMBERHOME "$work/amber12"
# Delete old files.
if (-d $AMBERHOME) then
mv $AMBERHOME $work/amber12-erase
rm -rf $work/amber12-erase &
endif
setenv DO_PARALLEL "mpirun -np 2"
#
cd $work
bunzip2 -c /home/users/${USER}/build/amber12/AmberTools12.tar.bz2 | tar xf -
bunzip2 -c /home/users/${USER}/build/amber12/Amber12.tar.bz2 | tar xf -
cd $AMBERHOME
foreach i (/home/users/${USER}/build/amber12/patches/Amber*/*)
patch -p0 < $i
end

```

```
#
# To get compiler version correctly, set LANG environment value.
setenv LANG C
# SSE_TYPES environment value means option "-ax${SSE_TYPES}", so unset it.
unsetenv SSE_TYPES
# If you use intel compiler version 12,
#   rism1d will be aborted and test of MPI fail.
source /opt/intel/Compiler/11.1/080/bin/iccvars.csh intel64
source /opt/intel/Compiler/11.1/080/bin/fortvars.csh intel64
# Create symbolic link for mpicc and mpif90 to become mpiicc and mpiifort respectively.
# Add option "-Wl,-rpath,/opt/intel..." in icc, icpc and ifort.set path=(/home/users/$USER/compiler/ccuv/intel-11.1 $path)
#
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
```