Compile Amber 7 and Amber 8 for opteron cluster

Hardware Environment: 24 nodes cluster of dual-opteron connected by myrinet

```
$ cat /proc/cpuinfo
processor       : 1
vendor_id       : AuthenticAMD
cpu family      : 15
model           : 5
model name      : AMD Opteron(tm) Processor 246
stepping        : 10
cpu MHz         : 2004.591
cache size      : 1024 KB
fpu             : yes
fpu_exception   : yes
cpuid level     : 1
wp              : yes
flags           : fpu vme de pse tsc msr pae mce cx8 apic sep mtrr pge mca cmov pat pse36 clflush mmx fxsr sse sse2
syscall nx mmxext lm 3dnowext 3dnow
bogomips        : 4005.88
TLB size        : 1024 4K pages
clflush size    : 64
cache_alignment : 64
address sizes   : 40 bits physical, 48 bits virtual
power management: ts fid vid ttp
......
```

Software Environment

1. Operating system: Linux-SuSE Professional 9.3 for x86-64 (kernel: 2.6.12-ck2)
2. Compiler: PGI 6.0
3. Message Passing: mpich-mx-1.2.6..0.94
4. Simulatoin packages: Amber 7 and Amber 8

Useful resource:

1. **Amber 7 and Amber 8 installation instruction (under $AMBERHOME/INSTALL)**
2. Compiling Amber 7: **http://amber.scripps.edu/cluster_info/compile_a7.html**
3. PGI guide to Amber: **http://www.pgroup.com/resources/amber/amber8_pgi52.htm**
4. PGI guide to MPICH: **http://www.pgroup.com/resources/mpich/mpich126_pgi60.htm**
5. Amber8 on Opteron: **http://amber.scripps.edu/amber8_opteron.pdf**
6. Amber8 Benchmarks: **http://amber.scripps.edu/amber8.bench1.html**

Install MPICH-MX

Microway (our cluster vendor) included a script in the MPICH-MX package to simplify the installation. The script is:

```
#!/bin/sh

# edit the next couple of lines:
# CC is the C compiler.
# F90 is the F90 compiler.
# FC is the F77 compiler.
# MX_HOME is the location of MX binary install directory.
# PREFIX if the location of MPICH-MX binary install directory.
# RSHCOMMAND is the remote execution program to use.

export CC=pgcc
export F77=pgf77
export F90=pgf90

export MX_HOME=/opt/mx
export PREFIX=/usr/local/mpich-mx
export RSHCOMMAND=rsh
```

```
export CFLAGS="-I${MX_HOME}/include"

#mxrpath="-Wl,-rpath,${MX_HOME}/lib32,-rpath,${MX_HOME}/lib64"
mxlibs="$mxrpath -L${MX_HOME}/lib32 -L${MX_HOME}/lib64 -lmyriexpress -lpthread"

./configure --with-device=ch_mx -prefix=$PREFIX -opt="-O"      \
            -lib="$mxlibs" \
                2>&1 | tee config-out.log

make 2>&1 | tee make.log

make install 2>&1 | tee install.log
```

However, this script installs MPICH-MX with the mixture of PGI compiler and GNU compiler, which will bring us lots of trouble later. Specifically, linking sander with the mpich-mx library will fail, giving out error messages like:

```
pgf90 -Bstatic -Mfree  -o sander trace.o lmod.o decomp.o icosasurf.o egb.o findmask.o pb_force.o sander.o cshf.o
noecalc.o noeread.o caldis.o calrate.o dinten.o drates.o indexn.o kmat.o pearsn.o plane.o remarc.o nmrcal.o nmrred.o
restal.o getnat.o nmrnrg.o modwt.o disnrg.o angnrg.o tornrg.o nmrprt.o nmrgrp.o nmrcms.o nmrcmf.o impnum.o
nmrsht.o at2res.o chklin.o opnmrg.o printe.o runmin.o ndvprt.o force.o rdparm.o mdread.o locmem.o runmd.o getcor.o
r6ave.o r6drv.o aveint.o degcnt.o corf.o threeb.o tripl.o nmrrad.o decnvh.o fastwt.o echoin.o parallel.o jnrg.o shake.o
ene.o mdwrit.o minrit.o set.o setmm.o dynlib.o mdfil.o nmlsrc.o ew_force.o ew_setup.o ew_box.o ew_bspline.o
ew_fft.o ew_direct.o ew_recip.o pcshift.o align.o rstack.o istack.o rfree.o rgroup.o random.o lsqfit.o amopen.o debug.o
ew_recip_reg.o ew_handle_dips.o ew_dipole_recip.o mexit.o new_time.o extra_pts.o thermo_int.o matinv.o assert.o
mmtsb.o mmtsb_client.o erfcfun.o veclib.o mdm.o pb_init.o constantph.o prn_dipoles.o  \
        ../lmod/lmod.a  \
        ../lapack/lapack.a ../blas/blas.a ../lib/nxtsec.o ../lib/sys.a
egb.o(.text+0x215c): In function `genborn_egb_':
_egb.f: undefined reference to `mpi_allreduce_'
egb.o(.text+0x45e2):_egb.f: undefined reference to `mpi_allreduce_'
sander.o(.text+0x34): In function `MAIN_':
_sander.f: undefined reference to `mpi_init_'
sander.o(.text+0x52):_sander.f: undefined reference to `mpi_comm_rank_'
sander.o(.text+0x66):_sander.f: undefined reference to `mpi_comm_size_'
sander.o(.text+0x75):_sander.f: undefined reference to `mpi_barrier_'
sander.o(.text+0xd8):_sander.f: undefined reference to `mpi_bcast_'
sander.o(.text+0x2a9):_sander.f: undefined reference to `mpi_bcast_'
sander.o(.text+0x2cd):_sander.f: undefined reference to `mpi_bcast_'
.....
```

I modifed the installation script to:

```
export CC=pgcc
export F77=pgf77
export F90=pgf90
export FC=pgf77
export CXX=pgCC
export CPP="pgCC -E"
export CXXFLAGS="-fast"
export F90FLAGS="-fast"
export FFLAGS="-fast"
export LDFLAGS="-fast"
export OPTFLAGS="-fast"

export MX_HOME=/opt/mx
export PREFIX=/home/myang/mpich-mx-pgi
export RSHCOMMAND=rsh


export CFLAGS="-I${MX_HOME}/include -fast"

#mxrpath="-Wl,-rpath,${MX_HOME}/lib32,-rpath,${MX_HOME}/lib64"
mxlibs="$mxrpath -L${MX_HOME}/lib64 -lmyriexpress -lpthread"
```

```
./configure --disable-doc --with-device=ch_mx -prefix=$PREFIX -opt="-fast"      \
        -lib="$mxlibs" \
            2>&1 | tee config-out.log

make 2>&1 | tee make.log

make install 2>&1 | tee install.log
```

After the installation of MPICH-MX finished, go to $MPICH_HOME/etc directory, make sure the Fortran compiler are set to pgf77 or pgf90 in files mpif77.conf and mpif90.conf.

Note: Please compile the MPICH library and the AMBER package with the exact SAME compiler. That's the key of a successful installation.

Compile Amber 7:

Once you compiled MPICH-MX library in the right way, installation of Amber 7 will be quite straitforward. The key to success is the correct settings in your MACHINE file. I get a MACHINE file from http://amber.scripps.edu/cluster_info/Machine.pgf77_mpich, and modified this file to optimize for opteron CPU.

```
#! /bin/csh -f
setenv MPICH_HOME /home/myang/mpich-mx-pgi
setenv MPICH_INCLUDE $MPICH_HOME/include
setenv MPICH_LIBDIR $MPICH_HOME/lib
setenv MPICH_LIB mpich

setenv MACHINE "linux/FreeBSD/Windows PC"
setenv MACH Linux
setenv MACHINEFLAGS "-DMPI"

# CPP is the cpp for this machine
setenv CPP "/lib/cpp -traditional -I$MPICH_INCLUDE"
setenv CC "pgcc "
setenv LOADCC "pgcc "

# SYSDIR is the name of the system-specific source directory relative to src/*/
setenv SYSDIR Machines/standard

# COMPILER ALIASES:
setenv FC "mpif77"
setenv OPT_0 "-g -tp=k8-64 -Mnoframe"
setenv OPT_1 "-O2 -Munroll -tp=k8-64 -Mnoframe"
setenv OPT_2 "-O2 -Munroll -tp=k8-64 -Mnoframe"
setenv OPT_3 "-O2 -Munroll -tp=k8-64 -Mnoframe"


# LOADER/LINKER:
setenv LOAD "mpif77 "
setenv LOADLIB "-lm -L$MPICH_LIBDIR -l$MPICH_LIB  "

#  following appears to be the best we have found so far:
setenv G77_OPT "-O3 -m64 -malign-double -ffast-math -fomit-frame-pointer"

# little or no optimization:
setenv L0 "$FC -c $OPT_0"

# modest optimization (local scalar):
setenv L1 "$FC -c $OPT_1"

# high scalar optimization (but not vectorization):
setenv L2 "$FC -c $OPT_2"

# high optimization (may be vectorization, not parallelization):
```

setenv L3 "$FC -c $OPT_3"

 # ranlib, if it exists
setenv RANLIB ranlib

Notice that I also change"pgf77" to "mpif77" in my MACHINE file. Because if I used "pgf77" to compile sander, I got error messages like:

pgf77 -o sander sander.o cshf.o noecalc.o noeread.o caldis.o calrate.o dinten.o drates.o indexn.o kmat.o pearsn.o plane.o remarc .o nmrcal.o nmrred.o restal.o getnat.o nmrnrg.o modwt.o disnrg.o angnrg.o tornrg.o nmrprt.o nmrgrp.o nmrcms.o nmrcmf.o impnum.o nmrsht.o at2res.o chklin.o opnmrg.o printe.o runmin.o ndvprt.o force.o rdparm.o mdread.o locmem.o runmd.o newvel.o getcor.o r6av e.o r6drv.o aveint.o degcnt.o corf.o threeb.o tripl.o nmrrad.o decnvh.o fastwt.o echoin.o parallel.o jnrg.o shake.o ene.o mdwrit .o minrit.o set.o setmm.o dynlib.o mdfil.o nmlsrc.o ew_force.o ew_setup.o ew_box.o ew_bspline.o ew_fft.o ew_direct.o ew_recip.o pcshift.o align.o rstack.o istack.o grdmax.o rfree.o rgroup.o ddotp.o random.o lsqfit.o amopen.o debug.o ew_recip_reg.o ew_handl e_dips.o ew_dipole_recip.o mexit.o egb.o new_time.o extra_pts.o thermo_int.o reorderwat.o matinv.o decomp.o ../lapack/lapack.a .
./blas/blas.a ../lib/nxtsec.o /home/myang/amber7/src/Machines/standard/sys.a -lm -L/home/myang/mpich-mx-pgi/lib -lmpich
/home/myang/mpich-mx-pgi/lib/libmpich.a(finalize.o)(.text+0x86): In function `PMPI_Finalize':
finalize.c: undefined reference to `MX_ERRORS_RETURN'
/home/myang/mpich-mx-pgi/lib/libmpich.a(finalize.o)(.text+0x95):finalize.c: undefined reference to `mx_set_error_handler'
/home/myang/mpich-mx-pgi/lib/libmpich.a(mxmpi_send.o)(.text+0xde): In function `MPID_SendContig':
mxmpi_send.c: undefined reference to `mx_isend'
/home/myang/mpich-mx-pgi/lib/libmpich.a(mxmpi_send.o)(.text+0xe9):mxmpi_send.c: undefined reference to `mx_strerror'
/home/myang/mpich-mx-pgi/lib/libmpich.a(mxmpi_send.o)(.text+0x135):mxmpi_send.c: undefined reference to `mx_strerror'
/home/myang/mpich-mx-pgi/lib/libmpich.a(mxmpi_send.o)(.text+0x203): In function `MPID_IsendContig'
.....

These error messages appeared when I compiled Amber 8, and the same trick kick them away. Remember to add $MPICH_HOME/bin into your PATH!

Compile Amber 8:

Thanks to the excellent work of Amber developers. The installation of Amber 8 becomes easier than the previous versions. However, to successfully compile it with PGI compiler, you need to do some modification. Follow the instruction at http://www.pgroup.com/resources/amber/amber8_pgi60.htm. To compile pmemd, maybe it's necessary to change "**pgf90**" to "**mpif90**" in the **linux_opteron.pgf90.mpich file**.

Benchmarks:

It is said Intel compiler can give better performance, though the CPUs are from AMD, so I also tried to compile Amber package with Intel compiler on the same machine.

Factor IX, 90906 atoms. ($AMBERHOME/benchmarks/factor_ix)
cutoff = 8.0 angstrom, timestep = 0.0015 psec, 500 steps.

	RunMD Time (seconds)		
cpu number	PGI	Intel	pmemd (compiled with PGI)
1	959.4 (67.5*)	931.4	795.0 (81.5)
2	482.9 (134.2)	455.7	417.4 (155.3)
4	287.8 (225.2)	266.5	234.6 (276.2)
8	143.1 (452.8)	151.5	128.8 (503.1)
16	97.9 (661.9)	95.3	70.7 (916.6)

gb_mb, 2492 atoms. ($AMBERHOME/benchmarks/gb_mb) 100steps, timestep = 0.001ps

1	49.6
2	24.9
4	12.6
8	6.5

*: Number in parenthesis means ps/day.