Amber14-bf0 for PRIMERGY

ウェブページ

http://ambermd.org/

バージョン

Amber 14 + AmberTools 14 bugfix 2

ビルド環境

- Intel Compiler 13.1.1.163
- Intel MPI 4.1.0.030
- Intel MKL 2013.3.163
- NVIDIA CUDA 5.0

ビルドに必要なファイル

- Amber14.tar.bz2
- AmberTools14.tar.bz2
- http://ambermd.org/bugfixesat.htmlにあるパッチ

ビルド手順

```
#!/bin/csh -f
umask 022
# Working directory must be installed directory to work with mpi4py.
set work="/local/apl/pg/amber14-bf0"
set build="/home/users/${USER}/build/amber14"
setenv AMBERHOME "$work"
setenv CUDA_HOME /usr/local/cuda
setenv LD_LIBRARY_PATH "${LD_LIBRARY_PATH}:${AMBERHOME}/lib"
setenv MKL_HOME ${MKLROOT}
# Installed directory must be created by builder.
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
# mpd should be run before test.
setenv DO_PARALLEL "mpirun -np 2"
cd $AMBERHOME
bunzip2 -c ${build}/Amber14.tar.bz2 | tar xf -
bunzip2 -c ${build}/AmberTools14.tar.bz2 | tar xf -
```

```
mv amber14/* .
#rmdir amber14
#
# Apply patches if they exist.
#
foreach i (${build}/patches/AmberTools14)
foreach j ($i/*.? $i/*.??)
patch -p0 < $j
end
end
chmod 755 AmberTools/test/charmmlipid2amber/Run.charmmlipid2amber
#
echo "[GPU (SPFP) serial edition]"
./configure --no-updates -cuda gnu
make -j 16 install
make clean
echo "[GPU (SPFP) parallel edition]"
./configure --no-updates -mpi -cuda gnu
make -j 16 install
make clean

echo "[GPU (DPFP) serial edition]"
./configure --no-updates -cuda_DPFP gnu
make -j 16 install
make clean
echo "[GPU (DPFP) parallel edition]"
./configure --no-updates -mpi -cuda_DPFP gnu
make -j 16 install
make clean

# LANG must be C to get correct a compiler version.
setenv LANG C
# Environment variable SSE_TYPES is insignificant.
source /opt/intel/composer_xe_2013.3.163/bin/compilervars.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 -intelmpi intel
make -j 16 install
make test
make clean
#
cd $AMBERHOME
rm -rf src
rm -rf AmberTools/src
```