Amber14-bf11 for PRIMERGY

ウェブページ

http://ambermd.org/

バージョン

Amber 14 bugfix 11 + AmberTools 14 bugfix 26

ビルド環境

- Intel Compiler 15.0.2.164
- Intel MPI 5.0.3.048
- Intel MKL 2015.2.164
- NVIDIA CUDA 7.0

ビルドに必要なファイル

- Amber14.tar.bz2
- AmberTools14.tar.bz2
- http://ambermd.org/bugfixes14.htmlにあるパッチ
- http://ambermd.org/bugfixesat.htmlにあるパッチ
- cuda70.patch

パッチファイル

cuda70.patch

```
diff --git AmberTools/src/configure2 AmberTools/src/configure2
index f1a3cff..9a504b1 100755
--- AmberTools/src/configure2
+++ AmberTools/src/configure2
@@ -721,13 +721,13 @@
       echo "CUDA Version $cudaversion detected"
       echo "Configuring for SM2.0 and SM3.0 - warning does not support Maxwell (GM200/GM204) cards [e.g. GTX970/980
       nvccflags="$sm20flags $sm30flags"
-    elif [ "$cudaversion" = "6.5" ]; then
+    elif [ "$cudaversion" = "6.5" -o "$cudaversion" = "7.0" ]; then
       echo "CUDA Version $cudaversion detected"
       echo "Configuring for SM2.0, SM3.0 and SM5.0"
       nvccflags="$sm20flags $sm30flags $sm50flags"
     else
       echo "Error: Unsupported CUDA version $cudaversion detected."
-      echo "AMBER requires CUDA version == 5.0 .or. 5.5 .or. 6.0 .or. 6.5"
+      echo "AMBER requires CUDA version == 5.0 .or. 5.5 .or. 6.0 .or. 6.5 .or. 7.0"
       exit 1
     fi
     nvcc="$nvcc $nvccflags"
```

注意事項

AmberTools15 bugfix 3ではテストが通らないため、AmberTools14を用いた。

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-bf11"
set build="/home/users/${USER}/build/amber14-bf11"
source /opt/intel/composer_xe_2015.2.164/bin/compilervars.csh intel64
setenv AMBERHOME "$work"
```

```
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/Amber14 ${build}/patches/AmberTools14)
foreach j ($i/*.? $i/*.??)
patch -p0 < $j
end
end
patch -p0 < ${build}/patches/cuda70.patch
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.
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
mv AmberTools/src/FEW .
```

```
rm -rf AmberTools/src
mkdir AmberTools/src
mv FEW AmberTools/src/
```