DIRAC 23.0

ウェブページ

http://www.diracprogram.org/doku.php

バージョン

23.0

ビルド環境

- Intel oneAPI Compiler Classic 2022.2.1 (oneAPI 2022.3.1)
- Intel MKL 2022.2.1 (oneAPI 2022.3.1)

ビルドに必要なファイル

- DIRAC-23.0-Source.tgz
- openmpi-4.1.5.tar.gz
    - (デフォルトを 8 バイト整数にするために既存のものとは別にビルド)
- diff_memcon (see /apl/dirac/23.0/patches/diff_memcon)
    - 利用可能なメモリ量を増やすためのパッチです

```
--- src/gp/memory_control.F90.orig      2019-08-08 13:42:54.000000000 +0900
+++ src/gp/memory_control.F90   2019-08-08 13:44:14.000000000 +0900
@@ -110,10 +110,10 @@

           subroutine allocator_setmax_i8(size)
             integer(kind=8), intent(in) :: size
-            integer(kind=4)            :: max_mem_i4
+            integer(kind=8)            :: max_mem_i8

             if (size.le.0) then ! there are no limits so we use a large integer
-              max_mem = real(huge(max_mem_i4))*real(kreal)
+              max_mem = real(huge(max_mem_i8))*real(kreal)
             else
               max_mem = real(size)*real(kreal)
             endif
```

ビルド手順

```
#!/bin/sh

VERSION=23.0
INSTALL_PREFIX=/apl/dirac/23.0
```

```
# openmpi (8-byte integer)
OMPI_VERSION=4.1.5
OMPI_INSTALL_PREFIX=${INSTALL_PREFIX}/openmpi415_i8
OMPI_TARBALL=/home/users/${USER}/Software/OpenMPI/${OMPI_VERSION}/openmpi-
${OMPI_VERSION}.tar.gz
PBSROOT=/apl/pbs/22.05.11/

# dirac
BASEDIR=/home/users/${USER}/Software/DIRAC/${VERSION}
TARBALL=${BASEDIR}/DIRAC-${VERSION}-Source.tgz

PATCH_README=${BASEDIR}/README.patch
PATCH_MEMCONTROL=${BASEDIR}/diff_memcon

WORKDIR=/gwork/users/${USER}

PARALLEL=8
#------------------------------------------------------------------------
umask 0022

export LC_ALL=C
export LANG=C
export OMP_NUM_THREADS=1

ulimit -s unlimited

module -s purge
. ~/intel/oneapi/compiler/latest/env/vars.sh
module -s load mkl/2022.2.1

# openmpi (8-byte integer default)
cd ${WORKDIR}
if [ -d openmpi-${OMPI_VERSION} ]; then
  mv openmpi-${OMPI_VERSION} openmpi_erase
  rm -rf openmpi_erase &
fi

tar zxf ${OMPI_TARBALL}
cd openmpi-${OMPI_VERSION}
mkdir rccs-i8 && cd rccs-i8
CC=icc CXX=icpc FC=ifort FCFLAGS=-i8 CFLAGS=-m64 CXXFLAGS=-m64 \
  ../configure --prefix=${OMPI_INSTALL_PREFIX} \
               --with-tm=${PBSROOT} \
               --enable-mpi-cxx \
               --enable-mpi1-compatibility \
               --enable-mpi-fortran=usempi \
               --with-ucx
make -j ${PARALLEL} && make install && make check
```

```
# dirac
cd ${WORKDIR}
if [ -d DIRAC-${VERSION}-Source ]; then
  mv DIRAC-${VERSION}-Source DIRAC_erase
  rm -rf DIRAC_erase &
fi

export PATH="${OMPI_INSTALL_PREFIX}/bin:$PATH"
export LIBRARY_PATH="${OMPI_INSTALL_PREFIX}/lib:$LIBRARY_PATH"
export LD_LIBRARY_PATH="${OMPI_INSTALL_PREFIX}/lib:$LD_LIBRARY_PATH"

export DIRAC_TMPDIR=${WORKDIR}

tar zxf ${TARBALL}
cd DIRAC-${VERSION}-Source
patch -p0 < ${PATCH_MEMCONTROL}

python3 ./setup \
        --mpi \
        --fc=mpif90 \
        --cc=mpicc \
        --cxx=mpicxx \
        --mkl=parallel \
        --int64 \
        --python=python2 \
        --extra-fc-flags="-march=core-avx2 -I${OMPI_INSTALL_PREFIX}/lib" \
        --extra-cc-flags="-march=core-avx2" \
        --extra-cxx-flags="-march=core-avx2" \
        --prefix=${INSTALL_PREFIX} \
        build.rccs
cd build.rccs
make -j ${PARALLEL} && make install

# copy license and patch files
cp -f ../LICENSE ${INSTALL_PREFIX}
cp -f ${PATCH_README} ${INSTALL_PREFIX}
mkdir ${INSTALL_PREFIX}/patches
cp -f ${PATCH_MEMCONTROL} ${INSTALL_PREFIX}/patches

# prepare test results directories
mkdir ${INSTALL_PREFIX}/test_results
mkdir ${INSTALL_PREFIX}/test_results/serial
mkdir ${INSTALL_PREFIX}/test_results/parallel

# serial test
export DIRAC_MPI_COMMAND="mpirun -np 1"
make test
cp Testing/Temporary/* ${INSTALL_PREFIX}/test_results/serial
rm -f Testing/Temporary/*
```

```
# parallel test
export DIRAC_MPI_COMMAND="mpirun -np ${PARALLEL}"
make test
cp Testing/Temporary/* ${INSTALL_PREFIX}/test_results/parallel
rm -f Testing/Temporary/*

exit 0
```

テスト

失敗したテスト(serial)

```
The following tests FAILED:
      31 - fde_response_mag (Failed)
      42 - fde_response_shield (Failed)
      46 - cc_restart (Failed)
     149 - laplace (Failed)
     172 - x_amfi (Failed)
     173 - pe_energy (Failed)
     174 - pe_response (Failed)
     175 - pe_exc (Failed)
     176 - pe_cpp (Failed)
```

失敗したテスト(parallel)

```
The following tests FAILED:
      21 - fscc_restart (Failed)
      31 - fde_response_mag (Failed)
      38 - dft_overlap_diagnostic (Failed)
      42 - fde_response_shield (Failed)
      46 - cc_restart (Failed)
     139 - lucita_short (Failed)
     149 - laplace (Failed)
     172 - x_amfi (Failed)
     173 - pe_energy (Failed)
     174 - pe_response (Failed)
     175 - pe_exc (Failed)
     176 - pe_cpp (Failed)
```

メモ

- テスト結果のコピーが /apl/dirac/23.0/test_results 以下にあります。
- gcc 10, 11 はビルドに dirac のビルドに失敗する
- gcc 8, 9 と intel 2022.2.1 については甲乙つけがたいが、intel 2022.2.1 の方がわずかに速度が出ているように見える(主に上記テストの結果より)
- intel compiler 2023.1.0 ではエラーが少し増えるため、今回は回避
- openmpi 3.1.6 よりも openmpi 4.1.5 の方がエラーが少しだけ少ない
    - 4ノードでの並列(512コア) HF 計算が正常に動くことは確認済
- aocc については dirac が未対応で、少なくとも大幅な修正が必要だと思われるため回避

- --python=python3 ではエラー(ascii, unicode 関連)が増えるため回避