## DIRAC 19.0

### ウェブページ

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

### バージョン

19.0

### ビルド環境

- Intel oneAPI Compiler Classic 2022.2.1 (oneAPI Base Toolkit 2022.3.1)

### ビルドに必要なファイル

- DIRAC-19.0-Source.tar.gz
- openmpi-3.1.6.tar.bz2
  - (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/19.0/patches/diff_memcon)
  - 利用可能なメモリ量を増やすためのパッチです

### ビルド手順

```
#!/bin/sh

VERSION=19.0
INSTALL_PREFIX=/apl/dirac/19.0

# openmpi (8-byte integer)
OMPI_VERSION=3.1.6
OMPI_INSTALL_PREFIX=${INSTALL_PREFIX}/openmpi316_i8
OMPI_TARBALL=/home/users/${USER}/Software/OpenMPI/${OMPI_VERSION}/openmpi-${OMPI
_VERSION}.tar.bz2
PBSROOT=/apl/pbs/22.05.11/

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

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/2022.2.1/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 jxf ${OMPI_TARBALL}
cd openmpi-${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 \
               --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}

for f in test/*/test; do
  if [ ! -d $f ]; then
    sed -i -e "s/env python/env python3/" $f
  fi
done
sed -i -e "s/python/python3/" test/runtest_dirac.py test/runtest_config.py

python3 ./setup \
        --mpi \
        --fc=mpif90 \
        --cc=mpicc \
        --cxx=mpicxx \
        --mkl=parallel \
        --int64 \
        --python=python3 \
        --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

# store test results
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/LastTest.log ${INSTALL_PREFIX}/test_results/serial
if [ -f Testing/Temporary/LastTestsFailed.log ]; then
  cp Testing/Temporary/LastTestsFailed.log ${INSTALL_PREFIX}/test_results/serial
fi

# parallel test
export DIRAC_MPI_COMMAND="mpirun -np ${PARALLEL}"
make test
cp Testing/Temporary/LastTest.log ${INSTALL_PREFIX}/test_results/parallel
if [ -f Testing/Temporary/LastTestsFailed.log ]; then
  cp Testing/Temporary/LastTestsFailed.log ${INSTALL_PREFIX}/test_results/parallel
fi

exit 0
```

## テスト

### 失敗したテスト(serial)

- 43 - fde_response_mag (Failed)
- 44 - fde_response_shield (Failed)
- 54 - mcscf_energy (Failed)
- 65 - eedm_mhyp_ensps_krci (Failed)
- 73 - bss_energy (Failed)
- 74 - pam_test (Failed)
- 129 - operators_mo_mtx_elements (Failed)
- 131 - spinrot (Failed)

### 失敗したテスト(parallel)

- 18 - polprp_ph (Failed)
- 43 - fde_response_mag (Failed)
- 44 - fde_response_shield (Failed)
- 46 - fscc_restart (Failed)
- 54 - mcscf_energy (Failed)
- 61 - krci_energy_q_corrections (Timeout)
- 65 - eedm_mhyp_ensps_krci (Failed)
- 73 - bss_energy (Failed)
- 74 - pam_test (Failed)
- 111 - lucita_short (Failed)
- 129 - operators_mo_mtx_elements (Failed)
- 131 - spinrot (Failed)

## メモ

- テスト結果については /apl/dirac/19.0/test_results を参照
- 前回は 43, 44, 54, 61 のテストではエラー無し
  - 43, 44 については数値エラー
  - 54, 61 については何が問題かわからず
  - インテルコンパイラを 2022.0.2 にしても問題変わらず
- gcc では未検証