

## DIRAC 19.0

### Webpage

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

### Version

19.0

### Build Environment

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

### Files Required

- DIRAC-19.0-Source.tar.gz
- openmpi-3.1.6.tar.bz2
  - ((8-byte integer version; built during the procedure below)
- diff\_memcon (see `/apl/dirac/19.0/patches/diff_memcon`)
  - to increase available memory amount

### Build Procedure

```
#!/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
```

## Tests

### Failed tests (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)

### Failed tests (parallel)

- 18 - polprp\_ph (Failed)
- 43 - fde\_response\_mag (Failed)
- 44 - fde\_response\_shield (Failed)
- 46 - fsc 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)

## Notes

- Please see `/apl/dirac/19.0/test_results` for results of test.
- In the [previous build](#), there were no errors for 43, 44, 54, 61.
  - 43, 44: numerical errors
  - 54, 61: what are the problems?
  - Switching to Intel Compiler 2022.0.2 does not help.
- Didn't try with gcc.