## DIRAC 19.0

## Webpage

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

## Version

19.0

## Build Environment

- Intel Compiler 19.1.2
  - ifort 19.1.2
  - icc 19.1.2
  - icpc 19.1.2
- Intel MKL 2020.0.2
- cmake 3.16.3

## Files Required

- DIRAC-19.0-Source.tar.gz
- openmpi-3.1.0.tar.bz2
  - (8-byte integer version; built during the procedure below)
- diff_memcon (see /local/apl/lx/dirac190/patches/diff_memcon)
  - to increase available memory amount

## Build Procedure

```
#!/bin/sh

VERSION=19.0
INSTALL_PREFIX=/local/apl/lx/dirac190

# openmpi (8-byte integer)
OMPI_VERSION=3.1.0
OMPI_INSTALL_PREFIX=${INSTALL_PREFIX}/openmpi310_i8
OMPI_TARBALL=/home/users/${USER}/Software/OpenMPI/${OMPI_VERSION}/openmpi-${OMPI_VERSION}.tar.bz2
PBSROOT=/local/apl/lx/pbs14

# 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=/work/users/${USER}

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

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

ulimit -s unlimited

module purge
module load intel/19.1.2
module load mkl/2020.0.2
module load cmake/3.16.3
```

```
# 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-psm2
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}

./setup --mpi \
        --fc=mpif90 \
        --cc=mpicc \
        --cxx=mpicxx \
        --mkl=parallel \
        --int64 \
        --extra-fc-flags="-xHost -I${OMPI_INSTALL_PREFIX}/lib" \
        --extra-cc-flags="-xHost" \
        --extra-cxx-flags="-xHost" \
        --prefix=${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
```

## Test results

### List of failed tests: serial version (mpirun -np 1)

- 20 - eomcc
- 65 - eedm_mhyp_ensps_krci
- 73 - bss_energy
- 74 - pam_test
- 129 - operators_mo_mtx_elements
- 131 - spinrot

### List of failed tests: parallel version (mpirun -np 8)

- 18 - polprp_ph
- 46 - fscc_restart
- 65 - eedm_mhyp_ensps_krci
- 73 - bss_energy
- 74 - pam_test
- 95 - mp2_srdft_energies (Timeout)
- 111 - lucita_short
- 129 - operators_mo_mtx_elements
- 131 - spinrot

## Notes

- Test results are available at /local/apl/lx/dirac190/test_resutls. (The output files for each test are not available.)
- Intel compiler version shows somewhat better performance than GCC one.
- OpenMPI 4.0.2 built failes on 71 - basis_input_scripted test additionally (reason "Timeout"). We thus employ OpenMPI 3.x.
- Test 18 (polprp_ph): Always failed for parallel runs.
- Test 20 (eomcc): Only serial test of int64 build always fails. (Numerical error). This happens both for Intel Compiler and GCC.
- Test 46 (fscc_restart): Always failed for parallel runs.
- Test 65 (eedm_mhyp_ensps_krci): Minor numerical error? Happens regardless of compiler type (intel/gnu).
- Test 73 (bss_energy): Due to the int64 specification?
- Test 74 (pam_test) Unknown error.
- Test 95 (mp2_srdft_energies) It always failed with "Timeout" for a parallel execution.
- Test 111 (lucita_short): Due to int64 specification? This error does not happen for serial run.
- Test 129 (operators_mo_mtx_elements): Another unknown error regardless of compiler type.
- Test 131 (spinrot): Only in case of Intel Compiler, some of values have been swapped.