

## DIRAC 18.0 for LX

### Webpage

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

### Version

18.0

### Build Environment

- ▶ Intel Compiler 2019.1.144
  - ▶ ifort 19.0.1.144
  - ▶ icc 19.0.1.144
  - ▶ icpc 19.0.1.144
- ▶ Intel MKL 2019.0.1
- ▶ cmake 3.8.2

### Files Required

- ▶ DIRAC-18.0-Source.tar.gz
- ▶ openmpi-3.1.0.tar.bz2
  - ▶ (special build is required to enable 8-bytes default integer size)

### Build Procedure

```
#!/bin/sh
VERSION=18.0
INSTALL_PREFIX=/local/apl/lx/dirac180

# 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
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/19.0.1
module load mkl/2019.0.1
module load cmake/3.8.2

# 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 xzf ${TARBALL}
cd DIRAC-${VERSION}-Source
./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

# serial test
export DIRAC_MPI_COMMAND="mpirun -np 1"
make test

# parallel test
export DIRAC_MPI_COMMAND="mpirun -np ${PARALLEL}"
make test

exit 0

```

## Important Notice

You must cite reference(s) listed in <http://www.diracprogram.org/doku.php?id=citation> when your result is published. Please check `/local/apl/lx/dirac180/LICENSE` file for more details.

## Notes

- ▶ MPI is enabled, 8-bytes integer is used by default.
- ▶ OpenMP is enabled only for MKL functions. (MPI/OpenMP hybrid parallelization is possible.)
  - ▶ Hybrid parallel run information at [http://www.diracprogram.org/doc/master/tutorials/hybrid\\_parallel\\_cc\\_run/...](http://www.diracprogram.org/doc/master/tutorials/hybrid_parallel_cc_run/...) may be useful.
- ▶ OpenMPI 4.x can't be used with intact code. (Some of MPI functions used in DIRAC are obsolete and not available for OpenMPI 4.x or later.)
  - ▶ (update) might be possible if openmpi-4.x was built with `--enable-mpi1-compatibility` flag?

In this MPI enabled version, following tests failed regardless of the intel compiler version (checked for intel17, intel18, and intel19).

- ▶ `general_property_krci` (Failed)
- ▶ `operators_mo_mtx_elements` (Failed)

If multiple process are used (`-np 2` or more), the following three tests also fail in addition to the above ones.

- ▶ `polprp_ph` (Failed)
- ▶ `mp2_srdft_energies` (Timeout)
- ▶ `lucita_short` (Failed)