

DIRAC 23.0

Webpage

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

Version

23.0

Build Environment

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

Files Required

- DIRAC-23.0-Source.tgz
- openmpi-4.1.5.tar.gz
 - (8-byte integer version; built during the procedure below)
- diff_memcon (see /apl/dirac/23.0/patches/diff_memcon)
 - (to increase the amount of available memory)

```
--- 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
```

Build Procedure

```
#!/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
```

Tests

List of failed tests: 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)

List of failed tests: parallel

The following tests FAILED:

- 21 - fsc 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)

Notes

- Copies of test results are available at `/apl/dirac/23.0/test_results`.
- gcc 10 and 11 failed to build dirac.
- Intel 2022.2.1 shows slightly better performance than gcc 8-9. (according to the time of tests)
- There were some more errors in intel compiler 2023.1.0 version.
- Open MPI 4.1.5 version shows slightly less errors than 3.1.5.
 - 4 nodes parallel HF calculation (512 MPI procs) seems to work.
- DIRAC does not seem to support AOCC.
- `--python=python3` version failed on some tests with ascii/unicode errors.