OpenMolcas v24.10

Webpage

https://gitlab.com/Molcas/OpenMolcas

Version

v24.10

Build Environment

- GCC 9.2.1
- Intel MKL 2023.2.0
- HPC-X 2.13 (Open MPI 4.1.5)

Files Required

- OpenMolcas.tar.gz (git cloned directory was tar-gzipped)
- ga-5.8.2.tar.gz
- drvefp.patch

```
--- drvefp.F90    2024-11-01 13:35:56.000000000 +0900
+++ drvefp.diff    2024-11-06 16:22:58.000000000 +0900
@@ -19,7 +19,7 @@
use EFP_Module, only: Coor_Type, EFP_Coors, EFP_Instance, FRAG_Type, nEFP_FRAGMENTS
use EFP, only: EFP_Add_Fragment, EFP_Add_Potential, EFP_Create, EFP_Get_Frag_Atom_Count, EFP_Prepare, &
               EFP_Set_Electron_Density_Field_FN, EFP_Set_Frag_Coordinates
-use Definitions, only: wp, iwp
+use Definitions, only: wp, iwp, u6

implicit none
logical(kind=iwp), intent(in) :: First
```

- molcas_electron_density_field_fn.patch

```
--- molcas_electron_density_field_fn.F90    2024-11-01 13:35:56.000000000 +0900
+++ molcas_electron_density_field_fn.diff    2024-11-06 16:27:09.000000000 +0900
@@ -63,6 +63,8 @@

Molcas_ELECTRON_DENSITY_FIELD_FN = EFP_RESULT_SUCCESS

+end function Molcas_ELECTRON_DENSITY_FIELD_FN
+
#elif ! defined (EMPTY_FILES)

! Some compilers do not like empty files
```

Build Procedure

GlobalArrays

```
#!/bin/sh
set -e

GA_VERSION=5.8.2
GA_DIR=/home/users/${USER}/Software/ga/${GA_VERSION}
GA_SOURCE=${GA_DIR}/v${GA_VERSION}.tar.gz

WORKDIR=/gwork/users/${USER}
INSTALLDIR=/apl/openmolcas/v24.10/ga-5.8.2

#-----------------------------------------------------------------------
if [ ! -f "${GA_SOURCE}" ]; then
```

```
  echo "Error: Source file ${GA_SOURCE} not found"
  exit 1
fi

umask 0022
ulimit -s unlimited
export LANG=
export LC_ALL=C
export OMP_NUM_THREADS=1

cd $WORKDIR
if [ -d ga-${GA_VERSION} ]; then
  echo "Removing existing build directory..."
  mv ga-${GA_VERSION} ga_tmp
  rm -rf ga_tmp &
fi

# Load required modules
echo "Loading required modules..."
module purge

module -s load gcc-toolset/9
module -s load mkl/2023.2.0
module -s load openmpi/4.1.5-hpcx/gcc9

# Quick check for MPI compiler
if ! command -v mpicc >/dev/null 2>&1; then
  echo "Error: MPI compilers not found after loading modules"
  exit 1
fi

# Extract source
echo "Extracting source code..."
tar zxf ${GA_SOURCE}
cd ga-${GA_VERSION}

# Set compilation environment
export F77=mpif90 F90=mpif90 FC=mpif90
export CC=mpicc CXX=mpicxx
export MPIF77=mpif90 MPICC=mpicc MPICXX=mpicxx
export GA_FOPT="-O3" GA_COPT="-O3" GA_CXXOPT="-O3"

# Build and install
echo "Running autogen..."
sh autogen.sh

echo "Configuring..."
./configure --with-blas8=-mkl \
        --with-scalapack8=-mkl \
        --with-openib \
        --enable-i8 \
        --prefix=${INSTALLDIR}

echo "Building with ${PARALLEL} parallel jobs..."
make -j ${PARALLEL}

echo "Installing..."
make install

echo "Running tests..."
make check

# Save build configuration
echo "Saving configuration log..."
cp config.log ${INSTALLDIR}

echo "Installation completed successfully"
```

OpenMolcas

```
#!/bin/sh

VERSION=v24.10
SOURCEDIR=/home/users/${USER}/Software/openmolcas/${VERSION}
TARBALL=${SOURCEDIR}/OpenMolcas.tar.gz
INSTALL_DIR=/apl/openmolcas/${VERSION}
GAROOT=${INSTALL_DIR}/ga-5.8.2
PARALLEL=1
WORKDIR=/gwork/users/${USER}
VERIFYTMP=/gwork/users/${USER}/openmolcas-tmp-${VERSION}-gcc9-openib

# Check if required files exist
if [ ! -f "${TARBALL}" ]; then
  echo "Error: Tarball not found at ${TARBALL}"
  exit 1
fi

PATCH=${SOURCEDIR}/cmakelists.patch
export GAROOT

#------------------------------------------------------------
umask 0022
ulimit -s unlimited
export LANG=
export LC_ALL=C
export MOLCAS_TIMELIM=1800

module purge
module -s load gcc-toolset/9
module -s load mkl/2023.2.0
module -s load openmpi/4.1.5-hpcx/gcc9

cd $WORKDIR || exit 1

if [ -d OpenMolcas ]; then
  mv OpenMolcas OpenMolcas_tmp
  rm -rf OpenMolcas_tmp &
fi

tar zxf ${TARBALL} || { echo "Failed to extract tarball"; exit 1; }
cd OpenMolcas || exit 1

Git submodule updates with error checking
for module in "External/libmsym" "External/efp" "External/libwfa"; do
  echo "Updating submodule: $module"
  git submodule update --init $module || { echo "Failed to update submodule: $module"; exit 1; }
done

sed -i -e "/environ/s/= 1/= '1'/" \
    -e "/environ/s/= opt\['parallel'\]/= str(opt['parallel'])/" \
    sbin/verify

cd src/integral_util/
patch < ${SOURCEDIR}/drvefp.patch
patch < ${SOURCEDIR}/molcas_electron_density_field_fn.patch
cd -

mkdir -p build && cd build || exit 1

export FC=mpif90
export CC=mpicc
export CXX=mpicxx
PYTHONEXE=/usr/bin/python3.6
PYTHONINC=/usr/include/python3.6
PYTHONLIB=/usr/lib64/python3.6
```

```
Check if Python executable exists
if [ ! -f "${PYTHONEXE}" ]; then
   echo "Error: Python executable not found at ${PYTHONEXE}"
   exit 1
fi

cmake .. -DCMAKE_INSTALL_PREFIX=${INSTALL_DIR} \
       -DMPI_Fortran_COMPILER=${FC} \
       -DMPI_C_COMPILER=${CC} \
       -DMPI_CXX_COMPILER=${CXX} \
       -DPython_EXECUTABLE=${PYTHONEXE} \
       -DPython_INCLUDE_DIR=${PYTHONINC} \
       -DPython_LIBRARY=${PYTHONLIB} \
       -DMPI=ON \
       -DGA=ON \
       -DOPENMP=ON \
       -DLINALG=MKL \
       -DHDF5=ON \
       -DTOOLS=ON \
       -DFDE=ON \
       -DEFPLIB=ON \
       -DMSYM=ON \
       -DNEVPT2=OFF \
       -DDMRG=OFF \
       -DWFA=ON || { echo "CMake configuration failed"; exit 1; }

make -j${PARALLEL} || { echo "Make failed"; exit 1; }

mkdir -p ${VERIFYTMP}
export OMP_NUM_THREADS=2
time ./pymolcas verify --parallel 4 --tmp ${VERIFYTMP}

make install || { echo "Installation failed"; exit 1; }

echo "Installation completed successfully"
```

Tests

Parallel version (4 MPI, 2 OpenMP):

- additional:221: A floating point exception occurred in process rank 2.
- additional:826: INTERNAL ERROR
- grayzone:898: Results are too different from the reference.

Notes

- Copy of testlog is available in /apl/openmolcas/v24.10/test_results.