Siesta 5.2.2

Webpage

https://gitlab.com/siesta-project/siesta

Version

5.2.2 (+ hdf5-1.14.5, NetCDF 4.9.2, NetCDF Fortran 4.6.1, libxc 6.2.2)

Build Environment

- GCC 13.1.1 (gcc-toolset-13)
- Intel MPI 2021.14.1
- OpenBLAS 0.3.29 (lp64)
- ScaLAPACK 2.2.2
- Python 3.9
    - rumael.yaml (pip3.9 install ruamel.yaml --user)

Files Required

- siesta-5.2.2.tar.gz
- wannier90-3.1.0.tar.gz
- hdf5-1.14.5.tar.gz
- netcdf-c-4.9.2.tar.gz
- netcdf-fortran-4.6.1.tar.gz
- libxc-6.2.2.tar.bz2
- (some of packages are downloaded in the procedure below)

Build Procedure

```
#!/bin/sh

SIESTA_VERSION=5.2.2
INSTDIR=/apl/siesta/5.2.2

WORKDIR=/gwork/users/${USER}
BASEDIR=/home/users/${USER}/Software/Siesta/${SIESTA_VERSION}
TARBALL=${BASEDIR}/siesta-${SIESTA_VERSION}.tar.gz

HDF5_VERSION=1.14.5
BASEDIR_HDF5=/home/users/${USER}/Software/HDF5/${HDF5_VERSION}
TARBALL_HDF5=${BASEDIR_HDF5}/hdf5-${HDF5_VERSION}.tar.gz
NETCDF_C_VERSION=4.9.2
NETCDF_F_VERSION=4.6.1
BASEDIR_NETCDF=/home/users/${USER}/Software/NETCDF
TARBALL_NETCDF_C=${BASEDIR_NETCDF}/c${NETCDF_C_VERSION}/netcdf-c-${NETCDF_C_VERSION}.tar.gz
TARBALL_NETCDF_F=${BASEDIR_NETCDF}/f${NETCDF_F_VERSION}/netcdf-fortran-${NETCDF_F_VERSION}.tar.gz
LIBXC_VERSION=6.2.2
BASEDIR_LIBXC=/home/users/${USER}/Software/libxc
TARBALL_LIBXC=${BASEDIR_LIBXC}/${LIBXC_VERSION}/libxc-${LIBXC_VERSION}.tar.bz2
WANNIER90_VERSION=3.1.0
BASEDIR_WANNIER90=/home/users/${USER}/Software/wannier90/${WANNIER90_VERSION}
TARBALL_WANNIER90=${BASEDIR_WANNIER90}/wannier90-${WANNIER90_VERSION}.tar.gz

PARALLEL=12

#-------------------------------------------------------------------------
umask 0022
ulimit -s unlimited

module -s purge
module -s load gcc-toolset/13
module -s load intelmpi/2021.14.1
```

```
module -s load openblas/0.3.29-lp64
module -s load scalapack/2.2.2-impi2021gcc-lp64

export LANG=C
export LC_ALL=C
export OMP_NUM_THREADS=1
#export I_MPI_HYDRA_TOPOLIB=ipl

# libxc

if [ ! -f ${INSTDIR}/exts/lib/libxc.a ]; then
 cd ${WORKDIR}
 if [ -d libxc-${LIBXC_VERSION} ]; then
   mv libxc-${LIBXC_VERSION} libxc-erase
   rm -rf libxc-erase &
 fi
 tar xf ${TARBALL_LIBXC}
 cd libxc-${LIBXC_VERSION}
 autoreconf -i
 ./configure --prefix=${INSTDIR}/exts
 make -j${PARALLEL}
 make -j${PARALLEL} check
 make install
fi

# hdf5

if [ ! -f ${INSTDIR}/exts/lib/libhdf5.a ]; then
 cd ${WORKDIR}
 if [ -d hdf5-${HDF5_VERSION} ]; then
   mv hdf5-${HDF5_VERSION} hdf5-erase
   rm -rf hdf5-erase &
 fi
 tar zxf ${TARBALL_HDF5}
 cd hdf5-${HDF5_VERSION}
 mkdir build && cd build
 cmake .. \
     -DCMAKE_INSTALL_PREFIX=${INSTDIR}/exts \
     -DHDF5_BUILD_FORTRAN=ON \
     -DHDF5_ENABLE_PARALLEL=ON \
     -DMPIEXEC_MAX_NUMPROCS=${PARALLEL}
 make -j${PARALLEL}
 make install
 make test # very long...
fi

export CC=mpicc
export CXX=mpicxx
export FC=mpif90
export F90=mpif90

export PATH="${INSTDIR}/exts/bin:${PATH}"
export CPATH="${INSTDIR}/exts/include:${CPATH}"
export LD_LIBRARY_PATH="${INSTDIR}/exts/lib:${LD_LIBRARY_PATH}"
export LIBRARY_PATH="${INSTDIR}/exts/lib:${LIBRARY_PATH}"

# netcdf-c

if [ ! -f ${INSTDIR}/exts/lib/libnetcdf.a ]; then
 cd ${WORKDIR}
 if [ -d netcdf-c-${NETCDF_C_VERSION} ]; then
   mv netcdf-c-${NETCDF_C_VERSION} netcdf-c-erase
   rm -rf netcdf-c-erase &
 fi
 tar zxf ${TARBALL_NETCDF_C}
 cd netcdf-c-${NETCDF_C_VERSION}
```

```
 LDFLAGS="-L${INSTDIR}/exts/lib" \
   ./configure --prefix=${INSTDIR}/exts \
               --enable-parallel-tests
 make -j${PARALLEL}
 make -j${PARALLEL} check
 make install
fi

# netcdf-f

if [ ! -f ${INSTDIR}/exts/lib/libnetcdff.a ]; then
 export FC="mpif90 -I/apl/oneapi/mpi/2021.14.1/include"
 cd ${WORKDIR}
 if [ -d netcdf-fortran-${NETCDF_F_VERSION} ]; then
   mv netcdf-fortran-${NETCDF_F_VERSION} netcdf-fortran-erase
   rm -rf netcdf-fortran-erase &
 fi
 tar zxf ${TARBALL_NETCDF_F}
 cd netcdf-fortran-${NETCDF_F_VERSION}

 LDFLAGS="-L${INSTDIR}/exts/lib" \
     ./configure --prefix=${INSTDIR}/exts \
                 --enable-parallel-tests
 make -j${PARALLEL}
 make -j${PARALLEL} check
 make install
fi

# siesta

cd ${WORKDIR}
if [ -d siesta-${SIESTA_VERSION} ]; then
 mv siesta-${SIESTA_VERSION} siesta-erase
 rm -rf siesta-erase
fi

tar zxf ${TARBALL}
cd siesta-${SIESTA_VERSION}

unset CC
unset CXX
unset FC
unset F90
export WANNIER90_PACKAGE=${TARBALL_WANNIER90}

mkdir build && cd build
cmake .. \
 -DCMAKE_INSTALL_PREFIX="${INSTDIR}" \
 -DCMAKE_PREFIX_PATH="${INSTDIR}/exts" \
 -DCMAKE_C_COMPILER=mpicc \
 -DCMAKE_CXX_COMPILER=mpicxx \
 -DCMAKE_Fortran_COMPILER=mpif90 \
 -DPython3_EXECUTABLE=/usr/bin/python3.9 \
 -DSIESTA_WITH_MPI=ON \
 -DBLAS_LIBRARY="-lopenblas -lscalapack" \
 -DLAPACK_LIBRARY=NONE \
 -DSCALAPACK_LIBRARY=NONE \
 -DNetCDF_PARALLEL=ON \
 -DNetCDF_ROOT="${INSTDIR}/exts" \
 -DSIESTA_WITH_OPENMP=OFF \
 -DSIESTA_WITH_DFTD3=ON \
 -DSIESTA_WITH_LIBXC=ON \
 -DSIESTA_WITH_ELSI=ON \
 -DSIESTA_WITH_WANNIER90=ON

make -j ${PARALLEL}
```

```
SIESTA_TESTS_VERIFY=1 ctest
make install
cp -r Testing/Temporary ${INSTDIR}/testlog

cd ../
cp -r Examples ${INSTDIR}
```

Tests

HDF5

Following tests did not run.

- 915 - H5REPACK-szip_individual (Disabled)
- 916 - H5REPACK-szip_all (Disabled)
- 933 - H5REPACK-all_filters (Disabled)
- 937 - H5REPACK-szip_copy (Disabled)
- 938 - H5REPACK-szip_remove (Disabled)
- 987 - H5REPACK-remove_all (Disabled)
- 988 - H5REPACK-deflate_convert (Disabled)
- 989 - H5REPACK-szip_convert (Disabled)

One test failed.

- 2930 - MPI_TEST_H5_f90_ph5_f90_filtered_writes_no_sel (Failed)

NetCDF-C, NetCDF-Fortran, libxc

All the tests passed.

Siesta

Copy of logfile can be found at /apl/siesta/5.2.2/testlog.

- 61 - siesta-02.SpinPolarization-fe_spin_mpi4[verify] (Failed)
- 63 - siesta-02.SpinPolarization-fe_spin_directphi_mpi4[verify] (Failed)
- 67 - siesta-02.SpinPolarization-fe_noncol_gga_mpi4[verify] (Failed)
- 71 - siesta-02.SpinPolarization-fe_noncol_sp_mpi4[verify] (Failed)
- 73 - siesta-03.SpinOrbit-FePt-X-X_mpi4[verify] (Failed)
- 87 - siesta-04.SCFMixing-chargemix_mpi4[verify] (Failed)

Notes

- Error of larger jobs when Intel MPI is used (reference:5.0.0 installation notes) is resolved by "export I_MPI_HYDRA_TOPOLIB=ipl"
  - This error would be related to resource management mechanism of RCCS system. This error may not happen on normal cluster system.
  - When the environment variable is added, message like "IPL WARN> IPL_init_numa_nodes: can not define numa node num" will be shown in the log file.
  - If "export I_MPI_HYDRA_TOPOLIB=ipl" is enabled in the procedure above, some HDF5 tests fail additionally (most probably due to the IPL_WARN> message).
  - Since the number of cases where this error occurs is expected to be limited, "unset I_MPI_HYDRA_TOPOLIB" may work in most cases.
- Intel MPI version is slightly faster than Open MPI (tested with 4.1.8) version.
- OpenBLAS version is slightly faster than MKL version.
- Not tested in detail with AOCC. There seems to be so many problems.
- Intel oneAPI compiler (icx,icpx,ifx) version failed with ~90 tests of Siesta (~30% of total). We thus didn't use it.
  - NOTE: some of calculations may be faster than GCC version. This may be very useful in some situation.
  - The performance of classic compiler (oneAPI 2023, icc+icpc+ifort) version is not so good as new one, although this didn't failed on tests.
- Python 3.9 and ruamel.yaml is necessary only upon tests. (ref:5.0.0 installation notes)