

[Siesta 5.0.0 MPI \(Intel MPI\)](#)

Webpage

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

Version

5.0.0 (+ELPA 2024.03.001, ELSI 2.9.1, NetCDF 4.9.2, NetCDF Fortran 4.6.1, libxc 6.2.2)

Build Environment

- GCC 11.2.1 (gcc-toolset-11)
- Intel MKL 2024.1
- Intel MPI 2021.11
- autoconf 2.72 (for ELPA)
- Python 3.9
 - `rumael.yaml` (`pip3.9 install rumael.yaml --user`)

Files Required

- `siesta-5.0.0.tar.gz`
- `netcdf-c-4.9.2.tar.gz`
- `netcdf-fortran-4.6.1.tar.gz`
- `libxc-6.2.2.tar.bz2`
- `elsi_interface-v2.9.1.tar.gz`
- `elpa-2024.03.001.tar.gz`
- `wannier90-3.1.0.tar.gz`
- `gnu_rccs.cmake` (for ELSI 2.9.1)

```
### GCC ###
```

```
SET(CMAKE_Fortran_COMPILER "mpif90" CACHE STRING "MPI Fortran compiler")
SET(CMAKE_C_COMPILER "mpicc" CACHE STRING "MPI C compiler")
SET(CMAKE_CXX_COMPILER "mpicxx" CACHE STRING "MPI C++ compiler")
```

```
SET(CMAKE_Fortran_FLAGS "-O3" CACHE STRING "Fortran flags")
SET(CMAKE_C_FLAGS "-O3 -std=c99" CACHE STRING "C flags")
SET(CMAKE_CXX_FLAGS "-O3 -std=c++11" CACHE STRING "C++ flags")
```

```
SET(ENABLE_PEXSI ON CACHE BOOL "Enable PEXSI")
SET(ENABLE_TESTS ON CACHE BOOL "Enable Fortran tests")
SET(ENABLE_C_TESTS ON CACHE BOOL "Enable C tests")
```

```
SET(LIB_PATHS "$ENV{MKLROOT}/lib/intel64" CACHE STRING "External library paths")
SET(LIBS "mkl_scalapack_lp64 mkl_gf_lp64 mkl_sequential mkl_core mkl_blacs_intelmpi_lp64 m dl"
  CACHE STRING "External libraries")
```

Build Procedure

ELSI (for PEXSI, not for ELPA)

```
#!/bin/sh

VERSION=2.9.1
INSTDIR=/apl/siesta/5.0.0-impi/exts

BASEDIR=/home/users/${USER}/Software/ELSI/${VERSION}
TARBALL=${BASEDIR}/elsi_interface-v${VERSION}.tar.gz

WORKDIR=/gwork/users/${USER}

MYTC_NAME=gnu_rccs.cmake
MYTC=${BASEDIR}/${MYTC_NAME}

PARALLEL=24
export LANG=C
```

```

export LC_ALL=C

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

cd ${WORKDIR}
if [ -d elsi_interface-v${VERSION} ]; then
  mv elsi_interface-v${VERSION} elsi-erase
  rm -rf elsi-erase &
fi

module -s purge
module -s load gcc-toolset/11
module -s load mkl/2024.1
module -s load intelmpi/2021.11

tar xf ${TARBALL}
cd elsi_interface-v${VERSION}
cp ${MYTC} toolchains

mkdir build && cd build
cmake .. \
  -DCMAKE_INSTALL_PREFIX=${INSTDIR} \
  -DCMAKE_TOOLCHAIN_FILE=./toolchains/${MYTC_NAME} \
  -DBUILD_SHARED_LIBS=ON

make -j ${PARALLEL}
make test
make install

```

ELPA

```

#!/bin/sh

ELPA_VERSION=2024.03.001
INSTDIR=/apl/siesta/5.0.0-impi/elpa
WORKDIR=/gwork/users/${USER}

BASEDIR=/home/users/${USER}/Software/ELPA/${ELPA_VERSION}
TARBALL=${BASEDIR}/elpa-${ELPA_VERSION}.tar.gz

PARALLEL=12

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

module -s purge
module -s load gcc-toolset/11
module -s load mkl/2024.1
module -s load intelmpi/2021.11
module -s load autoconf/2.72

export LANG=C
export LC_ALL=C

export FC=mpif90
export CC=mpicc
export CXX=mpicxx
export CFLAGS="-march=znver3"
# mkl_link_tool -opts -c gnu_f -p no --cluster_library=scalapack -m openmpi
export FCFLAGS="-m64 -I${MKLRROOT}/include"
# mkl_link_tool -libs -c gnu_f -p no --cluster_library=scalapack -m openmpi
export LDFLAGS="-L${MKLRROOT}/lib -lmkl_scalapack_lp64 -WI,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lmkl_blacs_intelmpi_lp64 -lpthread -lm -ldl"

cd ${WORKDIR}
if [ -d elpa-${ELPA_VERSION} ]; then
  mv elpa-${ELPA_VERSION} elpa-erase

```

```

rm -rf elpa-erase &
fi
tar xzf ${TARBALL}
cd elpa-${ELPA_VERSION}

./configure --prefix=${INSTDIR} \
            --disable-avx512-kernels
make -j ${PARALLEL}
make check
make install

```

Siesta

```

#!/bin/sh

SIESTA_VERSION=5.0.0
INSTDIR=/apl/siesta/5.0.0-impi

WORKDIR=/gwork/users/${USER}
BASEDIR=/home/users/${USER}/Software/Siesta/${SIESTA_VERSION}
TARBALL=${BASEDIR}/siesta-${SIESTA_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-
${NETCDF_F_VERSION}.tar.gz
WANNIER90_VERSION=3.1.0
BASEDIR_WANNIER90=/home/users/${USER}/Software/wannier90/${WANNIER90_VERSION}
TARBALL_WANNIER90=${BASEDIR_WANNIER90}/wannier90-${WANNIER90_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

PARALLEL=12

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

module -s purge
module -s load gcc-toolset/11
module -s load mkl/2024.1
module -s load intelmpi/2021.11

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

# netcdf-c

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 xzf ${TARBALL_NETCDF_C}
cd netcdf-c-${NETCDF_C_VERSION}

./configure --prefix=${INSTDIR}/exts
make -j${PARALLEL}
make -j${PARALLEL} check
make install

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-f

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 xzf ${TARBALL_NETCDF_F}
cd netcdf-fortran-${NETCDF_F_VERSION}

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

# libxc

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 -j24
make -j24 check
make install

# siesta

cd ${WORKDIR}
rm -rf netcdf-fortran-${NETCDF_F_VERSION} \
  netcdf-c-${NETCDF_C_VERSION} \
  libxc-${LIBXC_VERSION} &

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

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

unset CC
unset FC
export WANNIER90_PACKAGE=${TARBALL_WANNIER90}

mkdir build && cd build
cmake .. \
  -DCMAKE_INSTALL_PREFIX="${INSTDIR}" \
  -DCMAKE_PREFIX_PATH="${INSTDIR}/elpa:${INSTDIR}/exts" \
  -DCMAKE_C_COMPILER=mpicc \
  -DCMAKE_Fortran_COMPILER=mpif90 \
  -DPython3_EXECUTABLE=/usr/bin/python3.9 \
  -DSIESTA_WITH_MPI=ON \
  -DNetCDF_ROOT="${INSTDIR}/exts" \
  -DLAPACK_LIBRARY="-m64 -L${MKLRROOT}/lib -Wl,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl" \
  -DBLAS_LIBRARY="-m64 -L${MKLRROOT}/lib -Wl,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl" \
  -DSCALAPACK_LIBRARY="-lmkl_scalapack_lp64 -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lmkl_blacs_intelmpi_lp64 -lpthread -lm -ldl" \
  -DSIESTA_WITH_WANNIER90=ON \
  -DSIESTA_WITH_ELPA=ON \
  -DSIESTA_WITH_PEXSI=ON

```

```
make -j ${PARALLEL}
SIESTA_TESTS_VERIFY=1 ctest
make install
```

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

Tests

ELSI

All the tests have passed.

ELPA

Following tests failed.

- FAIL: validate_c_version_complex_double_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_c_version_real_double_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_c_version_complex_single_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_c_version_real_single_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL:
validate_c_version_complex_double_eigenvectors_2stage_default_kernel_random_explicit_default.sh
- FAIL: validate_c_version_complex_double_eigenvectors_2stage_default_kernel_random_default.sh
- FAIL:
validate_c_version_complex_single_eigenvectors_2stage_default_kernel_random_explicit_default.sh
- FAIL: validate_c_version_complex_single_eigenvectors_2stage_default_kernel_random_default.sh
- FAIL: validate_cpp_version_complex_double_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_cpp_version_real_double_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_cpp_version_complex_single_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_cpp_version_real_single_eigenvalues_2stage_default_kernel_analytic_default.sh
- FAIL: validate_cpp_version_complex_double_eigenvectors_2stage_default_kernel_random_default.sh
- FAIL:
validate_cpp_version_complex_single_eigenvectors_2stage_default_kernel_random_explicit_default.sh
- FAIL: validate_cpp_version_complex_single_eigenvectors_2stage_default_kernel_random_default.sh
- FAIL: validate_complex_double_eigenvalues_2stage_default_kernel_toeplitz_default.sh
- FAIL: validate_complex_single_eigenvalues_2stage_default_kernel_toeplitz_default.sh
- FAIL: validate_double_instance_default.sh
- FAIL: validate_real_2stage_banded_default.sh
- FAIL: validate_complex_2stage_banded_default.sh
- FAIL: validate_single_real_2stage_banded_default.sh
- FAIL: validate_single_complex_2stage_banded_default.sh

Siesta

(All the netcdf and libxc tests have passed.)

For Siesta, following tests failed with numerical error. Most ones are minor error. Although some of errors are bit large, changing compilers etc. could not improve the result.

- 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)
- 127 - siesta-08.GeometryOptimization-broyden_vc_mpi4[verify] (Failed)

Test logs are copied to /apl/siesta/5.0.0-impi/test_results.

Notes

- [Please check notes of Open MPI version.](#)