

Siesta 5.0.0 MPI (Intel MPI)

ウェブページ

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

バージョン

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

ビルド環境

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

ビルドに必要なファイル

- 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{MKLRROOT}/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")
```

ビルド手順

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${MKLROOT}/include"
# mkl_link_tool -libs -c gnu_f -p no --cluster_library=scalapack -m openmpi
export LDFLAGS="-L${MKLROOT}/lib -lmkl_scalapack_lp64 -Wl,--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 zxf ${TARBALL}
cd elpa-${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 zxf ${TARBALL_NETCDF_C}
cd netcdf-c-${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}
```

テスト

ELSI

すべてパス

ELPA

以下のテストで失敗

- 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

(netcdf, libxc についてはすべてパス)

siesta については以下のテストで数値エラー。ほとんどは軽微なエラー。一部で少し大きめな誤差が発生しているものの、コンパイラ等を変えても状況を改善させられず。

- 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)

テストログは /apl/siesta/5.0.0-impi/test_results 以下のコピーを保存しています。

メモ

- [Open MPI 版のメモをご確認ください。](#)
- (2025/2/13) export I_MPI_HYDRA_TOPOLIB=ipl で並列時の問題が解消することを確認。module ファイルを更新しました。