

Siesta 5.0.1 MPI (Intel MPI)

Webpage

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

Version

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

Build Procedure

- 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)
- ([netcdf](#), [libxc](#), [elpa](#), [pexsi](#) for 5.0.0 were also used for this version.)

Files Required

- siesta-5.0.1.tar.gz
- wannier90-3.1.0.tar.gz
- ([netcdf](#), [libxc](#), [elpa](#), [pexsi](#) for 5.0.0 were also used for this version.)

Build Procedure

```
#!/bin/sh

SIESTA_VERSION=5.0.1
INSTDIR=/apl/siesta/5.0.1-impi

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

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

# 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 FC
export WANNIER90_PACKAGE=${TARBALL_WANNIER90}

export LD_LIBRARY_PATH="${INSTDIR}/elpa/lib:${INSTDIR}/exts/lib:${LD_LIBRARY_PATH}"

mkdir build && cd build
cmake .. \
-DMAKE_INSTALL_PREFIX="${INSTDIR}" \
-DMAKE_PREFIX_PATH="${INSTDIR}/elpa:${INSTDIR}/exts" \
-DMAKE_C_COMPILER=mpicc \
-DMAKE_Fortran_COMPILER=mpif90 \
-DPython3_EXECUTABLE=/usr/bin/python3.9 \
-DSIESTA_WITH_MPI=ON \
-DNetCDF_ROOT="${INSTDIR}/exts" \
-DLAPACK_LIBRARY="-m64 -L${MKLROOT}/lib -Wl,--no-as-needed -lmkl_gf_lp64 -lmkl_sequential -lmkl_core -lpthread -lm -ldl" \
-DBLAS_LIBRARY="-m64 -L${MKLROOT}/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

Please check results for [version 5.0.0](#), since there are no remarkable differences with this version. Copied log files are available in `/apl/siesta/5.0.1-impi/test_results`.

Notes

- [Please check the page for version 5.0.0](#).
 - The installation is almost the same. `LD_LIBRARY_PATH` setting was added before `cmake` command.
 - `NetCDF`, `libxc`, `ELPA`, `PEXSI` for `siesta 5.0.0` were also used for this version. (Symbolic links "exts" and "elpa" were created before the procedure above.)
- (Although the output says "Version : unreleased 3852ac6d4 (2024-06-25)", this is version 5.0.1...)
- (Feb 13, 2025) `export I_MPI_HYDRA_TOPOLIB=ipl` was added to the module file to prevent errors upon parallel runs.