

Siesta 4.0.2 for LX

Webpage

<https://launchpad.net/siesta>

Version

4.0.2

Build Environment

- ▶ Intel Parallel Studio 2017 Update 8

Files Required

- ▶ siesta-4.0.2.tar.gz
- ▶ netcdf-c-4.6.3.tar.gz
- ▶ netcdf-fortran-4.4.4.tar.gz
- ▶ arch.make (Src/configure can be used alternatively)

```
.SUFFIXES:
.SUFFIXES: .f .F .o .a .f90 .F90

SIESTA_ARCH=rccs-intel17-mkl

FC=mpiifort
FC_SERIAL=ifort
FPP=${FC} -E -P
FFLAGS= -O2 -ip -xHost -fp-model source
RANLIB=ranlib
SYS=nag
LDFLAGS=
FCFLAGS_fixed_f=-fixed
FCFLAGS_free_f90=-free
FPPFLAGS_fixed_F=-fixed
FPPFLAGS_free_F90=-free
BLAS_LIBS=-mkl=sequential
LAPACK_LIBS=-mkl=sequential
BLACS_LIBS=L$(MKLRROOT)/lib/intel64 -lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64 -lmkl_sequential -lmkl_core -
lpthread -lm -ldl
SCALAPACK_LIBS=L$(MKLRROOT)/lib/intel64 -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64 -lmkl_intel_lp64 -
lmkl_sequential -lmkl_core -lpthread -lm -ldl
MPI_LIBS=
COMP_LIBS=
NETCDF_ROOT=$INSTDIR/netcdf
NETCDF_INCFLAGS=-I$(NETCDF_ROOT)/include
NETCDF_LIBS=$(NETCDF_ROOT)/lib/libnetcdf.a \
$(NETCDF_ROOT)/lib/libnetcdf.a -lcurl -lhdf5 -lhdf5_hl
MPI_INTERFACE=libmpi_f90.a
MPI_INCLUDE=.
FPPFLAGS= -DMPI -DCDF -DFC_HAVE_ABORT -DFC_HAVE_FLUSH
LIBS=$(NETCDF_LIBS) $(SCALAPACK_LIBS) $(BLACS_LIBS) $(LAPACK_LIBS) \
$(MPI_LIBS) $(COMP_LIBS)
FFLAGS_DEBUG=-g

#atom.o: atom.f
# $(FC) -c $(FFLAGS_DEBUG) $<
#electrostatic.o: electrostatic.f
# $(FC) -c $(FFLAGS_DEBUG) $<

.F.o:
$(FC) -c $(FFLAGS) $(INCFLAGS) $(FPPFLAGS) $(FPPFLAGS_fixed_F) $<
.F90.o:
$(FC) -c $(FFLAGS) $(INCFLAGS) $(FPPFLAGS) $(FPPFLAGS_free_F90) $<
.f.o:
$(FC) -c $(FFLAGS) $(INCFLAGS) $(FCFLAGS_fixed_f) $<
.f90.o:
$(FC) -c $(FFLAGS) $(INCFLAGS) $(FCFLAGS_free_f90) $<
```

Build Procedure

```
#!/bin/sh
VERSION=4.0.2
INSTDIR=/local/apl/lx/siesta402
WORKDIR=/work/users/${USER}
BASEDIR=/home/users/${USER}/Software/Siesta/${VERSION}
TARBALL=${BASEDIR}/siesta-${VERSION}.tar.gz
ARCHMAKE=${BASEDIR}/arch.make
```

```

NETCDF_C_VERSION=4.6.3
NETCDF_F_VERSION=4.4.4
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
PARALLEL=12 # NOTE: parallel make cannot be used for siesta
#-----
module purge
module load intel_parallelstudio/2017update8

export LANG=C
export LC_ALL=C
export FC=ifort
export CC=icc

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

./configure --prefix=${INSTDIR}/netcdf
make -j${PARALLEL}
# make -j${PARALLEL} check # can pass correctly
make install

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

./configure --prefix=${INSTDIR}/netcdf
make -j${PARALLEL}
## nf03_test & f03tst_open_mem fail due to hdf5 problem?
# make LDFLAGS="-L${INSTDIR}/netcdf/lib" -j${PARALLEL} check
make install

cd ${INSTDIR}
if [ -d siesta-${VERSION} ]; then
  mv siesta-${VERSION} siesta-erase
  rm -rf siesta-erase
fi
tar xzvf ${TARBALL}
mv siesta-${VERSION}/* .
rmdir siesta-${VERSION}

# hidoiyo...
echo >> Tests/OMM_h2o/OMM_h2o.fdf
echo >> Tests/OMM_si/OMM_si.fdf

mkdir bin # install dir

cd Obj
../Src/obj_setup.sh
cp ${ARCHMAKE} .

# build transiesta and run example
make transiesta && mv transiesta ${INSTDIR}/bin
cd ${INSTDIR}/Examples/TranSiesta/Elec && mkdir OUT_Test && cd OUT_Test
cp ../.
${INSTDIR}/bin/transiesta < elec.fast.fdf > elec.fast.out
cd ../Scat && mkdir OUT_TS_Test && cd OUT_TS_Test
cp ../.
cp ../Elec/OUT_Test/elec.fast.TSHS .
${INSTDIR}/bin/transiesta < scat.fast.fdf > scat.fast.out

# build siesta
cd ${INSTDIR}/Obj
make clean && make && mv siesta ${INSTDIR}/bin

# tests
cp -r Tests Tests.serial
cd Tests
make SIESTA="mpirun -np 4 ${INSTDIR}/bin/siesta" check >& make_check.log
cd ../ && mv Tests Tests.mpi && mv Tests.serial Tests && cd Tests
make SIESTA="${INSTDIR}/bin/siesta" check >& make_check.log

```

Notes

- ▶ Binary files are installed in "/local/apl/lx/siesta402/bin".
 - ▶ Corresponding module name is "siesta/4.0.2".
 - ▶ Sample scripts are available at "/local/apl/lx/siesta402/samples".
 - ▶ This version is licensed under GPLv3 unlike the former versions.
 - ▶ transiesta is also available (example works fine, at least).
 - ▶ As for compiler flags, -O2 is recommended for ifort. We thus employ that optimization level.
 - ▶ MPI version of intel18 + intelmpi(psxe18u2, psxe18u4) built did not work well.
 - ▶ (OpenMPI is not tested)
 - ▶ Newline is added to Tests/OMM_h2o/OMM_h2o.fdf and Tests/OMM_si/OMM_si.fdf at the end of file.
 - ▶ (Otherwise, tests cannot run correctly at least for ifort binaries.)
 - ▶ (Oct. 3, 2019 updated) Runtime library has to be 2017 version in some case; sample and modulefile are updated.
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