

# SIESTA

## Korištenje

Verzija	Modul
4.1.5	siesta/4.1.5

```
% module load siesta/4.1.5
% siesta
Siesta Version   : 4.1.5
Architecture     : unknown
Compiler version: ifort (IFORT) 19.0.0.117 20180804
Compiler flags   : mpifort -O2 -fPIC -fp-model source -qopenmp -I/apps/netcdf-fortran/4.5.3/include/
PP flags         : -DFC_HAVE_ABORT -DMPI -qopenmp -DNCDF -DNCDF_4 -DNCDF_PARALLEL -DSIESTA_METIIS -
DSIESTA_ELPA -I/apps/elpa/2020.11.001/avx2/include/elpa-2020.11.001/modules -DSIESTA_DIAG_2STAGE
Libraries        : libsiestaLAPACK.a libsiestaBLAS.a libfdict.a libncdf.a -qopenmp -mkl=paralleel -i8 -
lmkl_core -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64 -lmkl_sequential -lmkl_blas95_lp64 -L/apps/netcdf-c/4.
7.4/lib/ -L/apps/netcdf-fortran/4.5.3/lib/ -L/apps/hdf5/1.12.0/lib/ -lnetcdf -lnetcdf -lhdf5_fortran -lhdf5 -
lz -L/apps/metis/5.1.0/lib/ -lmetis -L/apps/elpa/2020.11.001/avx2/lib/ -lelpa
PARALLEL version
NetCDF-4 support
NetCDF-4 MPI-IO support
METIS ordering support
...
```

Primjer skripte za opis posla:

### siesta.sge

```
#$ -N siesta-parallel
#$ -q p28.q
#$ -pe *mpi 16
#$ -cwd

module load siesta/4.1.5

export OMP_NUM_THREADS=4

mpirun --bind-to socket -np 4 siesta < fe.fdf > fe.out
```

### Važno

Aplikacija se širi hibridno procesima (MPI paradigma) i dretvama (OpenMP paradigma). Varijabla okruženja `OMP_NUM_THREADS` definira koliko dretvi će svaki MPI proces kreirati. Iz tog razloga umnožak procesa i dretvi mora odgovarati zatraženom broju slotova definiranim u paralelnom okruženju. U primjeru je to  $16 = 4$  (MPI procesa)  $\times$   $4$  (OpenMP dretve)

## Instalacija

Programski paket SIESTA je pripremljen s kompajlerom Intel 2019, Intel MKL Scalapack i MPI implementacijom OpenMPI 3.0.0. Instalacija je obavljena pripremom pomoćnih biblioteka na koje se paket oslanja, dopremanjem izvornog koda, učitavanjem potrebnih modula za kompajler i MPI paralelizaciju te kompajliranjem samog paketa.

Priprema i instalacija se vršila prema uputstvima (uz male preinake specifične za Isabellu): <https://gitlab.com/siesta-project/siesta/-/releases/v4.1.5/downloads/siesta.pdf>

Izvorni kod se može pronaći na sjedištu: <https://gitlab.com/siesta-project/siesta>

# Priprema

## HD5

<https://www.hdfgroup.org/downloads/hdf5/source-code/>

### HDF5

```
module load mpi/openmpi3-intel-x86_64
CC=mpicc CXX=mpicxx FC=mpifort F90=mpif90 ./configure --prefix=/apps/hdf5/1.12.0 --enable-parallel --enable-
fortran
make -j8
make install
```

## NetCDF

<https://parallel-netcdf.github.io/>

### Parallel NetCDF

```
module load mpi/openmpi3-intel-x86_64
./configure --prefix=/apps/pnetcdf/1.12.2 --enable-shared
make -j8
make install
```

<https://www.unidata.ucar.edu/downloads/netcdf/>

### netcdf-c

```
module load mpi/openmpi3-intel-x86_64

LD_LIBRARY_PATH="/apps/hdf5/1.12.0/lib/:/apps/pnetcdf/1.12.2/lib:$LD_LIBRARY_PATH"
LIBS="-lhdf5_hl -lhdf5" LDFLAGS="-L/apps/hdf5/1.12.0/lib
-L/apps/pnetcdf/1.12.2/lib" CC=mpicc CPPFLAGS="-I/apps/hdf5/1.12.0/include
-I/apps/pnetcdf/1.12.2/include" CXX=mpicxx ./configure
--prefix=/apps/netcdf-c/4.7.4/ --enable-pnetcdf

make -j8
make install
```

### netcdf-fortran

```
module load mpi/openmpi3-intel-x86_64

LD_LIBRARY_PATH="/apps/netcdf-c/4.7.4/lib/:$LD_LIBRARY_PATH" CC=mpicc
CXX=mpicxx FC=mpifort F90=ifort CPPFLAGS="-I/apps/netcdf-c/4.7.4/include/"
LDFLAGS="-L/apps/netcdf-c/4.7.4/lib/" ./configure
--prefix=/apps/netcdf-fortran/4.5.3/

make -j8
make install
```

## METIS

<http://glaros.dtc.umn.edu/gkhome/metis/metis/download>

## metis

```
make config prefix=/apps/metis/5.1.0/ cc=icc
make install
```

## ELPA

<https://elpa.mpcdf.mpg.de/elpa-tar-archive>

## elpa

```
module load mpi/openmpi3-intel-x86_64

LIBS="-qopenmp -mkl=parallel -i8 -lmkl_core -lmkl_scalapack_lp64
-lmkl_blacs_openmpi_lp64 -lmkl_sequential -lmkl_blas95_lp64"
./configure --prefix=/apps/elpa/2020.11.001/avx2

make -j8
make install
```

## MUMPS

<http://mumps.enseeiht.fr/index.php?page=dwnld#form>

## MUMPS

```
module load mpi/openmpi3-intel-x86_64

cd MUMPS_5.3.5
cp Make.inc/Makefile.INTEL.PAR Makefile.inc
make all
cp -R lib/ include/ /apps/mumps/5.3.5/
```

## Kompajliranje i instalacija SIESTA

### Dopremanje izvornog koda i otpakiranje

```
wget -c https://gitlab.com/siesta-project/siesta/-/package_files/6659062/download -O siesta-4.1.5.tar.gz
tar -v -xzf siesta-4.1.5.tar.gz
```

### Priprema

```
cd siesta-4.1.5/Obj/
sh ../Src/obj_setup.sh
cp intel.make arch.make
module load mpi/openmpi3-intel-x86_64
```

Datoteku `arch.make` je potrebno editirati i dodati postavke za MPI paralelizaciju, Intel kompajler te povezivanje na pomoćne biblioteke:

## arch.make

```
# parallel compile @ Isabella
CC = mpicc
FPP = $(FC) -E -P
FC = mpifort
FC_SERIAL = ifort

FFLAGS = -O2 -fpIC -fp-model source -qopenmp

MPI_INTERFACE=libmpi_f90.a
MPI_INCLUDE=.
FPPFLAGS += -DMPI -qopenmp
LIBS += -qopenmp -mkl=parallel -i8 -lmkl_core -lmkl_scalapack_lp64 -lmkl_blacs_openmpi_lp64 -lmkl_sequential -
lmkl_blas95_lp64
LIBS += -L/apps/netcdf-c/4.7.4/lib/ -L/apps/netcdf-fortran/4.5.3/lib/ -L/apps/hdf5/1.12.0/lib/ -lnetcdff -
lnetcdf -lhdf5_fortran -lhdf5 -lz

# fdict
COMP_LIBS += libfdict.a
# ncdf
COMP_LIBS += libncdf.a
FPPFLAGS += -DNCDF -DNCDF_4 -DNCDF_PARALLEL
FFLAGS += -I/apps/netcdf-fortran/4.5.3/include/
# metis
LIBS += -L/apps/metis/5.1.0/lib/ -lmetis
FPPFLAGS += -DSIESTA_METIS
# elpa
LIBS += -L/apps/elpa/2020.11.001/avx2/lib/ -lelpa
FPPFLAGS += -DSIESTA_ELPA -I/apps/elpa/2020.11.001/avx2/include/elpa-2020.11.001/modules
# mumps
LIBS += -L/apps/mumps/5.3.5/lib/ -lmumps -lmumps_common -
lpord
FPPFLAGS += -DSIESTA_MUMPS
FFLAGS += -I/apps/mumps/5.3.5/include/
```

## Kompajliranje

```
make -j8
cp siesta /apps/siesta/4.1.5/avx2
```

## Instalacija pomoćnih alata

```
cd siesta-4.1.5/Util
find . -name Makefile -exec sed -i 's/$(LDFFLAGS)/$(LDFFLAGS) -qopenmp/g' {} \;
./build_all
find . -type f -executable -exec cp {} /apps/siesta/4.1.5/avx2 \;
ls /apps/siesta/4.1.5/avx2/
h2o/          eig2bxsf*      fractional*    ionplot.sh*   pblas_prb*   simple*       surf.py*
2dplot.py*   eigfat2plot*  get_chem_labels* macroave*     pi3*         simple_mpi_parallel* tbtrans*
Eig2DOS*     f2fmaster*    gnubands*     md2axsf*     plstm*       simple_mpi_serial*  ts2ts*
blacs_prb*   f2fslave*     gridld*       mixps*        plsts*       simple_pipes_parallel* tselecs.sh*
ccViz*       fat*          grid2d*       mprop*        protoNEB*    simple_pipes_serial*  vib2xsf*
clean_all.sh* fcbuild*     hs2hsx*       optical*      rho2xsf*     simple_sockets_parallel* vibra*
denchar*     fdf2grimme*  hsx2hs*       optical_input* sies2arc*    simple_sockets_serial* xv2xsf*
driver*      fmpdos*       int_explorer* para*         siesta*      spin_texture*
```