

Installation of OpenMX

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2015/03/30

Download

1. Download the latest version of OpenMX

```
% wget http://www.openmx-square.org/openmx3.7.tar.gz  
% tar openmx3.7.tar.gz
```

2. Download the latest batch

```
% wget http://www.openmx-square.org/bugfixed/15Feb21/patch3.7.10.tar.gz  
% cp ./patch3.7.10.tar.gz openmx3.7/source  
% cd openmx3.7/source  
% tar zxvf patch3.7.10.tar.gz
```

3. Install

Installation of OpenMX Ver.3.7

1. Set 3 parameters CC, FC, and LIB in
`openmx3.7/source/makefile` **according the system in**
use

CC: C compiler

FC: Fortran compiler

LIB: FFT, LAPACK and BLAS libraries

2. Compile

```
% make
```

3. Install

```
% make install
```

4. If successful, OpenMX executable file will be created in

```
openmx3.7/work/openmx
```

Settings of CC, FC, and LIB

FFTROOT=/path/to/fft/folder (FFT library path)

LBSROOT=/path/to/lapack/and/blas/folder (LAPACK and BLAS library path)

openmp_flag = -openmp (for Intel compilers)

openmp_flag = -fopenmp (for GNU compilers)

openmp_flag = -mp -Dnosse (for PGI compilers)

fortran_lib = -lifcore (for Intel compilers)

fortran_lib = -lgfortran (for GNU compilers)

fortran_lib = -pgf90libs (for PGI compilers)

CC=mpicc -O3 openmp_flag ¥

-I/\$(FFTROOT)/include ¥

-I/\$(LBSROOT)/include

FC=mpif90 -O3 -I/\$(LBSROOT)/include

LIB=-L/\$(FFTROOT)/lib -lfftw ¥

-L/\$(LBSROOT)/lib -llapack -lblas ¥

fortran_lib

Setting Sample 1: Intel Compilers and MKL Library

FFTRoot=/usr/local/fftw3 (FFT library path)
LBSRoot=/opt/intel/mkl (MKL library path)
openmp_flag = -openmp (for Intel compilers)
fortran_lib = -lifcore (for Intel compilers)

```
CC=mpicc -O3 -openmp ¥  
    -I/$(FFTRoot)/include ¥  
    -I/$(LBSRoot)/include  
FC=mpiifort -O3 -I/$(LBSRoot)/include  
LIB=-L/$(FFTRoot)/lib -lfftw3 ¥  
    -L/$(LBSRoot)/lib/intel64 -lmkl_intel_lp64 ¥  
    -lmkl_intel_thread -lmkl_core -lpthread ¥  
    -lifcore
```

Setting Sample 2: PGI Compilers and ACML Library

FFTRoot=/usr/local/fftw3 (FFT library path)
LBSRoot=/usr/local/acml/gnu64 (ACML library path)
openmp_flag = -mp -Dnosse (for PGI compilers)
fortran_lib = -pgf90libs (for PGI compilers)

CC=mpicc -O3 -mp -Dnosse ¥
-I/\$(FFTRoot)/include ¥
-I/\$(LBSRoot)/include
FC=mpif90 -O3 -I/\$(LBSRoot)/include
LIB=-L/\$(FFTRoot)/lib -lfftw3 ¥
-L/\$(LBSRoot)/lib/ -lacml ¥
-pgf90libs

Setting Sample 3: GNU Compilers and MKL Library

FFTRoot=/usr/local/fftw3 (FFT library path)
LBSRoot=/opt/intel/mkl (MKL library path)
openmp_flag = -fopenmp (for GNU compilers)
fortran_lib = -lgfortran (for GNU compilers)

```
CC=mpicc -O3 -fopenmp ¥  
    -I/$(FFTRoot)/include ¥  
    -I/$(LBSRoot)/include  
FC=mpif90 -O3 -I/$(LBSRoot)/include  
LIB=-L/$(FFTRoot)/lib -lfftw3 ¥  
    -L/$(LBSRoot)/lib/intel64 -lmkl_intel_lp64 ¥  
    -lmkl_intel_thread -lmkl_core -lpthread ¥  
    -lgfortran
```

Setting Sample 4: GNU Compilers and ACML Library

FFTRoot=/usr/local/fftw3 (FFT library path)
LBSRoot=/usr/local/acml/gnu64 (ACML library path)
openmp_flag = -fopenmp (for GNU compilers)
fortran_lib = -lgfortran (for GNU compilers)

CC=mpicc -O3 -fopenmp ¥
-I/\$(FFTRoot)/include ¥
-I/\$(LBSRoot)/include
FC=mpif90 -O3 -I/\$(LBSRoot)/include
LIB=-L/\$(FFTRoot)/lib -lfftw3 ¥
-L/\$(LBSRoot)/lib/ -lacml ¥
-lgfortran

Useful Commands

- **Show the compilers in use**

```
%mpicc -compile-info    (for MPICH)
%mpicc -help            (for OpenMPI)
```

- **Search for the Fortran library**

```
/usr/bin/ld: cannot find -lifcore (for Intel compilers)
/usr/bin/ld: cannot find -lpgf90  (for PGI compilers)
/usr/bin/ld: cannot find -lgfortran (for GNU compilers)
```

First search for its location

```
%which ifort          (for Intel compilers)
/opt/intel/fce/10.0.026/bin/ifort
%which pgf90          (for PGI compilers)
/opt/pgi/linux86-64/7.0/bin/pgf90
%which gfortran       (for GNU compilers)
/usr/bin/gfortran
```

Then add it to LIB

```
LIB= ... -L/opt/intel/fce/10.0.026/lib -lifcore (for Intel compilers)
LIB= ... -L/opt/pgi/linux86-64/7.0/lib -pgf90libs (for PGI compilers)
LIB= ... -L/usr/lib -lgfortran (for GNU compilers)
```

Frequently Encountered Error Messages (1)

- **No such file or directory (*.o files)**

```
gcc: openmx.o: No such file or directory
gcc: openmx_common.o: No such file or directory
.....
```

OR

```
icc: error #10236: File not found: 'elpa1.o'
icc: error #10236: File not found: 'solve_evp_real.o'
icc: error #10236: File not found: 'solve_evp_complex.o'
.....
```

- **Possible causes: (1) `openmp_flag` is not correctly set, OR, (2) `mpicc` AND/OR `mpif90` are not correctly set**

- **Solutions**

- (1) **Check `openmp_flag`**

- `openmp_flag = -openmp` (for Intel compilers)

- `openmp_flag = -fopenmp` (for GNU compilers)

- `openmp_flag = -mp -Dnosse` (for PGI compilers)

- (2) **Check `mpicc` and `mpif90` (not `mpicc` but `mpiicc`, `mpipgcc`; not `mpif90` but `mpiifort`, `mpifc77`, `mpipgf77`, `mpipgf90`)**

Frequently Encountered Error Messages (2)

- **Cannot find MPI Fortran library**

```
elpa1.o: In function `elpa1_mp_tridiag_real_':  
elpa1.f90:(.text+0x2b7): undefined reference to `mpi_comm_rank_'  
elpa1.f90:(.text+0x2d6): undefined reference to `mpi_comm_size_'  
elpa1.f90:(.text+0x2f5): undefined reference to `mpi_comm_rank_'  
elpa1.f90:(.text+0x314): undefined reference to `mpi_comm_size_'  
.....
```

- **Cause: As OpenMX uses the C compiler for linking, the MPI Fortran library is required**

- **Solution**

- **Add MPI Fortran library to LIB**

```
LIB = ... -lmpi_f77 -lmpi_f90 -lifcore
```

Frequently Encountered Error Messages (3)

- **Cannot find OpenMP library**

```
/libmkl_intel_thread.a(dgeqrf_par.o): In function `mkl_lapack_dgeqrf':  
__tmp_par_dgeqrf_omp.f:(.text+0x730): undefined reference to  
`__kmpc_critical'  
__tmp_par_dgeqrf_omp.f:(.text+0x833): undefined reference to `__kmpc_flush'  
__tmp_par_dgeqrf_omp.f:(.text+0x85c): undefined reference to `__kmpc_flush'  
__tmp_par_dgeqrf_omp.f:(.text+0xa32): undefined reference to `__kmpc_flush'  
.....  
libmkl_intel_thread.a(zher2k_drv.o): In function `mkl_blas_zher2k':  
../../../../../../blas/thread/32e/level3/zher2k.c:(.text+0x66b): undefined  
reference to `__kmpc_global_thread_num'  
../../../../../../blas/thread/32e/level3/zher2k.c:(.text+0x68b): undefined  
reference to `__kmpc_ok_to_fork'  
../../../../../../blas/thread/32e/level3/zher2k.c:(.text+0x6aa): undefined  
reference to `__kmpc_push_num_threads'
```

- **Cause: The C compiler could not locate the OpenMP library for linking**

- **Solution**

- **Add the OpenMP library to LIB**

```
LIB = ... -liomp5 -lpthread
```

Frequently Encountered Error Messages (4)

- **Cannot find MKL library**

```
/usr/bin/ld: cannot find -lmkl_intel_lp64
collect2: ld returned 1 exit status
make: *** [openmx] Error 1
```

- **Cause: The C compiler could not locate the MKL library when linking**

- **Solution**


























- **Add the MKL library to LIB**

```
LIB=-L/$(FFTRoot)/lib -lfftw3 ¥
-L/$(MKLROOT)/lib/intel64 -Wl,--start-group ¥
$(MKLROOT)/lib/intel64/libmkl_lapack95_lp64.a ¥
$(MKLROOT)/lib/intel64/libmkl_intel_lp64.a ¥
$(MKLROOT)/lib/intel64/libmkl_intel_thread.a ¥
$(MKLROOT)/lib/intel64/libmkl_core.a -Wl,--end-group ¥
-lifcore
```

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