

INSTALLATION PROCEDURE

#####

VASP-5.4.4.pl2

#####

Source file :- **vasp.5.4.4.pl2.tgz**

#tar -xvf vasp.5.4.4.pl2.tgz

#cd vasp.5.4.4.pl2

#module load compiler/intel/2018.2.199

#module load gnu8/8.3.0

#cp arch/makefile.include.linux_intel makefile.include

#####

#vi makefile.include

Precompiler options

**CPP_OPTIONS= -DHOST=\"LinuxIFC\" **

**-DMPI -DMPI_BLOCK=8000 **

**-Duse_collective **

**-DscLAPACK **

**-DCACHE_SIZE=4000 **

**-Davoidalloc **

**-Duse_bse_te **

**-Dtbdyn **

-Duse_shmem

CPP = fpp -f_com=no -free -w0 \$\$FUFFIX \$\$SUFFIX \$(CPP_OPTIONS)

FC = **mpiifort # With mpiifort Intel compiler**

FCL = **mpiifort -mkl=sequential -lstdc++ # With mpiifort Intel compiler**

FREE = -free -names lowercase

FFLAGS = -assume byterecl -w

OFLAG = -O2

```
OFLAG_IN = $(OFLAG)
DEBUG    = -O0
MKLROOT  = /opt/ohpc/pub/compiler/intel/2018_2/compilers_and_libraries_2018.2.199/linux/mkl/
MKL_PATH = $(MKLROOT)/lib/intel64
BLAS     =
LAPACK   = -L${MKL_PATH} -lmkl_scalapack_lp64 -lmkl_lapack95_lp64
BLACS    = -L${MKL_PATH} -lmkl_blacs_intelmpi_lp64
SCALAPACK = ${MKL_PATH}/libmkl_scalapack_lp64.a $(BLACS)
```

```
OBJECTS  = fftmpi.o fftmpi_map.o fft3dlib.o fftw3d.o
INCS     = -I$(MKLROOT)/include/fftw
LLIBS    = $(SCALAPACK) $(LAPACK) $(BLAS)
OBJECTS_O1 += fftw3d.o fftmpi.o fftmpi.o
OBJECTS_O2 += fft3dlib.o
```

```
# For what used to be vasp.5.lib
```

```
CPP_LIB  = $(CPP)
FC_LIB   = $(FC)
CC_LIB   = icc
CFLAGS_LIB = -O
FFLAGS_LIB = -O1
FREE_LIB = $(FREE)
```

```
OBJECTS_LIB= linpack_double.o getshmem.o
```

```
# For the parser library
```

```
CXX_PARS = icpc
LIBS     += parser
LLIBS    += -Lparser -lparser -lstdc++
```

```
# Normally no need to change this
```

```

SRCDIR = ../../src
BINDIR = ../../bin

#=====

# GPU Stuff

CPP_GPU = -DCUDA_GPU -DRPROMU_CPROJ_OVERLAP -DUSE_PINNED_MEMORY -DCUFFT_MIN=28 -
UscaLAPACK

OBJECTS_GPU = fftmpiw.o fftmpi_map.o fft3dlib.o fftw3d_gpu.o fftmpiw_gpu.o

CC = icc
CXX = icpc

CFLAGS = -fPIC -DADD_ -Wall -openmp -DMAGMA_WITH_MKL -DMAGMA_SETAFFINITY -
DGPUSHMEM=300 -DHAVE_CUBLAS

CUDA_ROOT ?= /usr/local/cuda/

NVCC := $(CUDA_ROOT)/bin/nvcc -ccbin=icc

CUDA_LIB := -L$(CUDA_ROOT)/lib64 -lnvToolsExt -lcudart -lcuda -lcufft -lcublas

GENCODE_ARCH := -gencode=arch=compute_30,code=\"sm_30,compute_30\" \
                -gencode=arch=compute_35,code=\"sm_35,compute_35\" \
                -gencode=arch=compute_60,code=\"sm_60,compute_60\"

MPI_INC = $(I_MPI_ROOT)/include64/

#####

make std
make gam
make ncl

Then.

ls -lrt bin | awk '{print $0}END{print NR " files found"}

```

Note: -

1. Inside the Job submission script file please mention “`module load compiler/intel/2018.2.199` and `module load gnu8/8.3.0`”.