### 安装大体可以分成3步：安装Intel编译器、编译libdmy.a和编译VASP主程序

1安装Intel编译器略

注意在编译器组件选择中要选上（默认是没选上的），clustering tools，否则会找不到libmkl\_scalapack\_lp64.a和libmkl\_scalapack\_ilp64.a。如果安装时没有选择，可以重新运行安装程序，modify即可。不要卸载重装！

2 编译libdmy.a

cp makefile.linux\_ifc\_P4 makefile

vi makefile

|  |
| --- |
| # C-preprocessor  CPP = icc -E -P -C $\*.F >$\*.f  FC=ifort  CFLAGS = -O  FFLAGS = -O0 -FI  FREE = -FR  DOBJ = preclib.o timing\_.o derrf\_.o dclock\_.o diolib.o dlexlib.o drdatab.o |

make

输出中会提示错误，论坛上说似乎可以忽略。输出如下：

|  |
| --- |
| ifort -O0 -FI -FR -c preclib.f  cc -O -c timing\_.c  cc -O -c derrf\_.c  cc -O -c dclock\_.c  ifort -O0 -FI -FR -c diolib.f  ifort -O0 -FI -FR -c dlexlib.f  ifort -O0 -FI -FR -c drdatab.f  ifort -O0 -FI -c lapack\_double.f  lapack\_double.f(10179): remark #5140: Unrecognized directive  CDIR$ NEXTSCALAR  -------------------------^  lapack\_double.f(10181): remark #5140: Unrecognized directive  CDIR$ NEXT SCALAR  --------------------------^  lapack\_double.f(20692): remark #5140: Unrecognized directive  CDIR$ NEXTSCALAR  -------------------------^  lapack\_double.f(20694): remark #5140: Unrecognized directive  CDIR$ NEXT SCALAR  --------------------------^  lapack\_double.f(20706): remark #5140: Unrecognized directive  CDIR$ NEXTSCALAR  ----------------------------^  lapack\_double.f(20708): remark #5140: Unrecognized directive  CDIR$ NEXT SCALAR  -----------------------------^  lapack\_double.f(20733): remark #5140: Unrecognized directive  CDIR$ NEXTSCALAR  -------------------------^  lapack\_double.f(20735): remark #5140: Unrecognized directive  CDIR$ NEXT SCALAR  --------------------------^  ifort -O0 -FI -c linpack\_double.f  rm libdmy.a  rm: cannot remove `libdmy.a': No such file or directory  make: [libdmy.a] Error 1 (ignored)  ar vq libdmy.a preclib.o timing\_.o derrf\_.o dclock\_.o diolib.o dlexlib.o drdatab.o  ar: creating libdmy.a  a - preclib.o  a - timing\_.o  a - derrf\_.o  a - dclock\_.o  a - diolib.o  a - dlexlib.o  a - drdatab.o |

3编译VASP主程序

cp arch/makefile.include.linux\_intel makefile.include

vi makefile.include

红色部分是所做的修改

|  |
| --- |
| # Precompiler options  CPP\_OPTIONS= -DHOST=\"LinuxIFC\"\  -DMPI -DMPI\_BLOCK=8000 \  -Duse\_collective \  -DscaLAPACK \  -DCACHE\_SIZE=4000 \  -Davoidalloc \  -Duse\_bse\_te \  -Dtbdyn \  -Duse\_shmem  CPP = fpp -f\_com=no -free -w0 $\*$(FUFFIX) $\*$(SUFFIX) $(CPP\_OPTIONS)  FC = mpif90  FCL = mpiifort -mkl=sequential -lstdc++  FREE = -free -names lowercase  FFLAGS = -assume byterecl –w -heap-arrays 64  OFLAG = -O2  OFLAG\_IN = $(OFLAG)  DEBUG = -O0  MKLROOT = /home1/lijia/intel/compilers\_and\_libraries/linux/mkl  MKL\_PATH = $(MKLROOT)/lib/intel64  BLAS = -L$(MKL\_PATH) -lmkl\_intel\_lp64 -lmkl\_sequential -lmkl\_core -lpthread  LAPACK = -L$(MKL\_PATH) -lmkl\_intel\_lp64 -lmkl\_sequential -lmkl\_core -lpthread  BLACS = -L$(MKL\_PATH) -lmkl\_blacs\_intelmpi\_lp64  SCALAPACK = $(MKL\_PATH)/libmkl\_scalapack\_lp64.a $(MKL\_PATH)/libmkl\_scalapack\_ilp64.a $(BLACS)  OBJECTS = fftmpiw.o fftmpi\_map.o fft3dlib.o fftw3d.o  INCS =-I$(MKLROOT)/include/fftw  LLIBS = $(SCALAPACK) $(LAPACK) $(BLAS)  OBJECTS\_O1 += fftw3d.o fftmpi.o fftmpiw.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/ |