

# VASP6 GPU ??

## VASP6 GPU?N?? ?????

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3. vasp vasp gpu openacc cuda  
 vasp6.2 openacc

[https://www.vasp.at/wiki/index.php/OpenACC\\_GPU\\_port\\_of\\_VASP](https://www.vasp.at/wiki/index.php/OpenACC_GPU_port_of_VASP)

## ????

Openacc gpu Vasp6 NVIDIA HPC-SDK PGI's Compilers & Tools (version  
>=19.10) vasp NVIDIA HPC-SDK **20.9**  
 vasp bug

4. NVIDIA HPC-SDK 20.9

<https://developer.nvidia.com/nvidia-hpc-sdk-209-downloads>

wget tarball  
 nvidia-smi cuda  
 version >=10.0

5. HPC-SDK 20.9

`/usr/software/nv-hpcsdk`

```
export NVARCH=`uname -s`_`uname -m`;
export NVCOMPILERS=/usr/software/nv-hpcsdk #
export PATH=$NVCOMPILERS/$NVARCH/20.9/compilers/bin:$PATH
export MANPATH=$MANPATH:$NVCOMPILERS/$NVARCH/20.9/compilers/man
export LD_LIBRARY_PATH=$NVCOMPILERS/$NVARCH/20.9/compilers/lib/:$LD_LIBRARY_PATH
export PATH=$NVCOMPILERS/$NVARCH/20.9/comm_libs/mpi/bin/:$PATH
```

gpu vasp6 bashrc bashrc  
intel mpirun

????

NVIDIA HPC-SDK 20.9 CUDA Toolkit, QD,  
NCCL, FFTW, HPC-SDK

FFTW nvhpc-sdk hpc-sdk  
GNU intel

/fs00/software/fftw/3.3.8-ips2019u5

???

vasp6.2

```
cp arch/makefile.include.linux_nv_acc makefile.include`
```

```
which nvfortran | awk -F /compilers/bin/nvfortran '{ print $1 }'
```

nvfortran nv-hpc-sdk

##### **vasp**##### **openacc+openmp**####

**makefile.include.linux\_nv\_acc+omp+mkl**## **nccl**## **openacc**

##### **openmp**

##### **openmp**

##### **makefile.include.linux\_nv\_acc**

#####

makefile.include#####

makefile.include#####

```
#Precompiler options
```

```
CPP_OPTIONS= -DHOST=\"LinuxPGI\" \  
             -DMPI -DMPI_BLOCK=8000 -DMPI_INPLACE -Duse_collective \  
             -DscalAPACK \  
             -DCACHE_SIZE=4000 \  
             -Davoidalloc \  
             -Dvasp6 \  
             -Duse_bse_te \  
             -Dtbdyn \  
             -Dqd_emulate \  
             -Dflock_dblbuf \  
             -D_OPENACC \  
             -DUSENCCL -DUSENCCLP2P
```

```
CPP          = nvfortran -mpreprocess -mfree -mextend -E $(CPP_OPTIONS) *$(SUFFIX) >  
              *$(SUFFIX)
```

```
FC           = mpif90 -acc -gpu=cc60,cc70,cc80,cuda11.0
```

```
FCL          = mpif90 -acc -gpu=cc60,cc70,cc80,cuda11.0 -c++libs
```

```
FREE         = -mfree
```

```
FFLAGS       = -Mbackslash -Mlarge_arrays
```

```
OFLAG        = -fast
```

```

DEBUG      = -Mfree -O0 -traceback

#Specify your NV HPC-SDK installation, try to set NVR00T automatically
NVR00T    =$(shell which nvfortran | awk -F /compilers/bin/nvfortran '{ print $1 }')
#or set NVR00T manually
#NVHPC      ?= /opt/nvidia/hpc_sdk
#NVVERSION  = 20.9
#NVR00T     = $(NVHPC)/Linux_x86_64/$(NVVERSION)

#Use NV HPC-SDK provided BLAS and LAPACK libraries
BLAS       = -lblas
LAPACK     = -llapack

BLACS      =
SCALAPACK  = -Mscalapack

CUDA       = -cudalib=cublas,cusolver,cufft,nccl -cuda

LLIBS      = $(SCALAPACK) $(LAPACK) $(BLAS) $(CUDA)

#Software emulation of quadruple precson
QD         = $(NVR00T)/compilers/extras/qd                #□□□□□□□□
LLIBS      += -L$(QD)/lib -lqdmmod -lqd
INCS       += -I$(QD)/include/qd

#Use the FFTs from fftw
FFTW       = /fs00/software/fftw/3.3.8-ips2019u5          #□□fftw□□□□□□□□□□
LLIBS      += -L$(FFTW)/lib -lfftw3
INCS       += -I$(FFTW)/include

OBJECTS    = fftmpi.o fftmpi_map.o fftw3d.o fft3dlib.o

#Redefine the standard list of 01 and 02 objects
SOURCE_01  := pade_fit.o
SOURCE_02  := pead.o

#For what used to be vasp.5.lib
CPP_LIB    = $(CPP)
FC_LIB     = nvfortran

```

```
CC_LIB      = nvc
CFLAGS_LIB = -O
FFLAGS_LIB = -O1 -Mfixed
FREE_LIB    = $(FREE)
```

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

```
#For the parser library
CXX_PARS    = nvc++ --no_warnings
```

```
#Normally no need to change this
SRCDIR      = ../../src
BINDIR      = ../../bin
```

```
#####
```

```
module load ips/2019u5 ######fftw#####
export NVARCH=`uname -s`_`uname -m`;
export NVCOMPILERS=/usr/software/nv-hpcsdk
export PATH=$NVCOMPILERS/$NVARCH/20.9/compilers/bin:$PATH
export MANPATH=$MANPATH:$NVCOMPILERS/$NVARCH/20.9/compilers/man
export LD_LIBRARY_PATH=$NVCOMPILERS/$NVARCH/20.9/compilers/lib/:$LD_LIBRARY_PATH
export PATH=$NVCOMPILERS/$NVARCH/20.9/comm_libs/mpi/bin/:$PATH
```

```
/usr/software/nv-hpcsdk  nv-hpc-sdk#####
```

```
make std gam ncl
```

```
##### openacc##### make gpu##### vasp_std
##### GPU#####
```

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1. nccl openacc gpu .

2. INCAR NCORE openacc 1.

3.INCAR NSIM KPAR

GPU NSIM cpu

GPU

VASP

Revision #8  
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