

# ????

□□□□

- [GNU](#)
- [Intel](#)
- [NVIDIA](#)
- [AMD](#)
- [Python](#)
- [Golang](#)
- [Open MPI](#)
- [Tcl/TK](#)
- [□□□□](#)
- [VASP6 GPU □□](#)
- [Quantum Espresso](#)
- [NAMD](#)
- [OOMMF](#)
- [Mumax3](#)
- [□□□□](#)
- [Singularity Image](#)
- [gnuplot](#)
- [OVITO](#)
- [Vim](#)
- [Zsh](#)
- [AlphaFold 2](#)
- [AlphaFold 3](#)
- [RoseTTAFold](#)
- [ParallelFold 2](#)

# GNU

## GNU Compiler Collection

Name	Path	Module
GNU Compiler Collection (GCC) 12.1.0 & GNU Binutils 2.38	/fs00/software/gcc/12.1.0	gcc/12.1.0
GNU Compiler Collection (GCC) 11.3.0 & GNU Binutils 2.36.1	/fs00/software/gcc/11.3.0	gcc/11.3.0
GNU Compiler Collection (GCC) 10.5.0 & GNU Binutils 2.34	/fs00/software/gcc/10.5.0	gcc/10.5.0
GNU Compiler Collection (GCC) 9.5.0 & GNU Binutils 2.32	/fs00/software/gcc/9.5.0	gcc/9.5.0
GNU Compiler Collection (GCC) 8.5.0 & GNU Binutils 2.30	/fs00/software/gcc/8.5.0	gcc/8.5.0
GNU Compiler Collection (GCC) 7.5.0 & GNU Binutils 2.28.1	/fs00/software/gcc/7.5.0	gcc/7.5.0
GNU Compiler Collection (GCC) 6.5.0 & GNU Binutils 2.26.1	/fs00/software/gcc/6.5.0	gcc/6.5.0
GNU Compiler Collection (GCC) 5.4.0	/fs00/software/gcc/5.4.0	gcc/5.4.0

## GNU Make

Name	Path	Module
GNU Make 4.3	/fs00/software/make/4.3	make/4.3
GNU Make 4.2.1	/fs00/software/make/4.2.1	make/4.2.1
GNU Make 4.2	/fs00/software/make/4.2	make/4.2

## GNU Scientific Library

Name	Compiler	Path	Module
GNU Scientific Library (GSL) 2.7.1	GCC 12.1.0	/fs00/software/gsl/2.7.1-gcc12.1.0	gsl/2.7.1-gcc12.1.0
GNU Scientific Library (GSL) 2.5	GCC 8.3.0	/fs00/software/gsl/2.5-gcc8.3	gsl/2.5-gcc8.3

# GNU C Library

Name	Compiler	Path	Module
GNU C Library (glibc) 2.36	GCC 12.1.0	/fs00/software/glibc/2.36-gcc12.1.0	glibc/2.36-gcc12.1.0
GNU C Library (glibc) 2.30	GCC 9.2.0	/fs00/software/glibc/2.30-gcc9.2.0	glibc/2.30-gcc9.2.0

# GNU Binutils

Name	Compiler	Path	Module
GNU Binutils 2.38	GCC 12.1.0	/fs00/software/binutils/2.38-gcc12.1.0	binutils/2.38-gcc12.1.0
GNU Binutils 2.27	GCC 5.4.0	/fs00/software/binutils/2.27-gcc5.4.0	binutils/2.27-gcc5.4.0

# Intel

## Intel oneAPI

Name	Path	MODULEPATH
Intel oneAPI Base Toolkit 2024.0.1 Intel HPC Toolkit 2024.0.1	/fs00/software/intel/oneapi2024.0	/fs00/software/modulefiles/oneapi/2024.0

## Intel Parallel Studio

Name	Path	Module
Intel Parallel Studio XE 2020 Update 2 Cluster Edition	/fs00/software/intel/ps2020u2	ips/2020u2
Intel Parallel Studio XE 2019 Update 5 Cluster Edition	/fs00/software/intel/ps2019u5	ips/2019u5
Intel Parallel Studio XE 2018 Update 4 Cluster Edition	/fs00/software/intel/ps2018u4	ips/2018u4
Intel Parallel Studio XE 2017 Update 6 Cluster Edition	/fs00/software/intel/ps2017u6	ips/2017u6
Intel Parallel Studio XE 2017 Update 2 Cluster Edition	/fs00/software/intel/ps2017u2	ips/2017u2
Intel Parallel Studio XE 2016 Update 4 Cluster Edition	/fs00/software/intel/ps2016u4	ips/2016u4
Intel Parallel Studio XE 2015 Update 6 Cluster Edition	/fs00/software/intel/ps2015u6	ips/2015u6
Intel Cluster Studio XE 2013 Service Pack 1 (SP1) Update 1	/fs00/software/intel/cs2013sp1u1	ics/2013sp1u1
Intel Cluster Studio XE 2013	/fs00/software/intel/cs2013	ics/2013
Intel Parallel Studio XE 2011 SP1 Update 3	/fs00/software/intel/ps2011sp1u3	ips/2011sp1u3

## Intel Distribution for Python

Name	Path
Intel Distribution for Python 2.7 2019 Update 5	/fs00/software/intel/ps2019u5/intelpython2
Intel Distribution for Python 3.6 2019 Update 5	/fs00/software/intel/ps2019u5/intelpython3

Name	Path
Intel Distribution for Python 2.7 2018 Update 3	/fs00/software/intel/python2018u3/intelpython2
Intel Distribution for Python 3.6 2018 Update 3	/fs00/software/intel/python2018u3/intelpython3
Intel Distribution for Python 2.7 2017 Update 3	/fs00/software/intel/python2017u3/intelpython2
Intel Distribution for Python 3.5 2017 Update 3	/fs00/software/intel/python2017u3/intelpython3

# NVIDIA

## CUDA Toolkit

Name	Path	Module
CUDA Toolkit 12.3.1	/fs00/software/cuda/12.3.1	cuda/12.3.1
CUDA Toolkit 12.0.0	/fs00/software/cuda/12.0.0	cuda/12.0.0
CUDA Toolkit 11.8.0	/fs00/software/cuda/11.8.0	cuda/11.8.0
CUDA Toolkit 11.2.0	/fs00/software/cuda/11.2.0	cuda/11.2.0
CUDA Toolkit 10.2.89	/fs00/software/cuda/10.2.89	cuda/10.2.89
CUDA Toolkit 10.1.243	/fs00/software/cuda/10.1.243	cuda/10.1.243
CUDA Toolkit 10.0.130	/fs00/software/cuda/10.0.130	cuda/10.0.130
CUDA Toolkit 9.2.148	/fs00/software/cuda/9.2.148	cuda/9.2.148
CUDA Toolkit 9.0.176 with Patch 3	/fs00/software/cuda/9.0.176	cuda/9.0.176
CUDA Toolkit 8.0 GA2 8.0.61 with Patch 2	/fs00/software/cuda/8.0.61	cuda/8.0.61

## cuDNN

Name	CUDA	Path	Module
cuDNN v8.9.7.29	12.x	/fs00/software/cudnn/8.9.7.29-cuda12	cudnn/8.9.7.29-cuda12
cuDNN v8.9.7.29	11.x	/fs00/software/cudnn/8.9.7.29-cuda11	cudnn/8.9.7.29-cuda11
cuDNN v8.7.0.84	11.x	/fs00/software/cudnn/8.7.0.84-cuda11	cudnn/8.7.0.84-cuda11
cuDNN v8.7.0.84	10.2	/fs00/software/cudnn/8.7.0.84-cuda10	cudnn/8.7.0.84-cuda10
cuDNN v8.1.1.33	11.2	/fs00/software/cudnn/11.2-v8.1.1.33	cudnn/11.2-v8.1.1.33
cuDNN v8.2.2.26	10.2	/fs00/software/cudnn/10.2-v8.2.2.26	cudnn/10.2-v8.2.2.26
cuDNN v7.6.5.32	10.2	/fs00/software/cudnn/10.2-v7.6.5.32	cudnn/10.2-v7.6.5.32

Name	CUDA	Path	Module
cuDNN v7.6.4.38	10.1	/fs00/software/cudnn/10.1-v7.6.4.38	cudnn/10.1-v7.6.4.38
cuDNN v7.6.5.32	10.0	/fs00/software/cudnn/10.0-v7.6.5.32	cudnn/10.0-v7.6.5.32
cuDNN v7.1.4	9.2	/fs00/software/cudnn/9.2-v7.1.4	cudnn/9.2-v7.1.4
cuDNN v7.1.4	9.0	/fs00/software/cudnn/9.0-v7.1.4	cudnn/9.0-v7.1.4
cuDNN v7.0.5	8.0	/fs00/software/cudnn/8.0-v7.0.5	cudnn/8.0-v7.0.5
cuDNN v6.0	8.0	/fs00/software/cudnn/8.0-v6.0	cudnn/8.0-v6.0
cuDNN v5.1	8.0	/fs00/software/cudnn/8.0-v5.1	cudnn/8.0-v5.1

## HPC SDK

Name	Path	MODULEPATH
HPC SDK 23.11	/fs00/software/nvhpc/23.11	/fs00/software/nvhpc/23.11/modulefiles
HPC SDK 22.11	/fs00/software/nvhpc/22.11	/fs00/software/nvhpc/22.11/modulefiles
HPC SDK 21.3	/fs00/software/nvhpc/21.3	/fs00/software/nvhpc/21.3/modulefiles
HPC SDK 20.9	/fs00/software/nvhpc/20.9	/fs00/software/nvhpc/20.9/modulefiles

## HPC-X

Name	CUDA	Path	MODULEPATH
HPC-X 2.17.1	12.x	/fs00/software/hpcx/2.17.1-cuda12	/fs00/software/hpcx/2.17.1-cuda12/modulefiles

## NCCL

Name	CUDA	Path	Module
NCCL 2.19.3	12.3	/fs00/software/nccl/2.19.3-cuda12.3	nccl/2.19.3-cuda12.3

Name	CUDA	Path	Module
NCCL 2.16.2	12.0	/fs00/software/nccl/2.16.2-cuda12.0	nccl/2.16.2-cuda12.0
NCCL 2.16.2	11.8	/fs00/software/nccl/2.16.2-cuda11.8	nccl/2.16.2-cuda11.8
NCCL 2.16.2	11.0	/fs00/software/nccl/2.16.2-cuda11.0	nccl/2.16.2-cuda11.0
NCCL v2.5.6	10.2	/fs00/software/nccl/10.2-v2.5.6	nccl/10.2-v2.5.6
NCCL v2.4.8	10.1	/fs00/software/nccl/10.1-v2.4.8	nccl/10.1-v2.4.8

# TensorRT

Name	CUDA	cuDNN	Path	Module
TensorRT 8.6.1.6	12.0		/fs00/software/tensorrt/8.6.1.6-cuda12.0	tensorrt/8.6.1.6-cuda12.0
TensorRT 8.6.1.6	11.8		/fs00/software/tensorrt/8.6.1.6-cuda11.8	tensorrt/8.6.1.6-cuda11.8
TensorRT 8.5.2.2	11.8	8.6	/fs00/software/tensorrt/8.5.2.2-cuda11.8-cudnn8.6	tensorrt/8.5.2.2-cuda11.8-cudnn8.6
TensorRT 8.5.2.2	10.2	8.6	/fs00/software/tensorrt/8.5.2.2-cuda10.2-cudnn8.6	tensorrt/8.5.2.2-cuda10.2-cudnn8.6
TensorRT 8.2.0.6	11.4	8.2	/fs00/software/tensorrt/8.2.0.6-cuda11.4-cudnn8.2	tensorrt/8.2.0.6-cuda11.4-cudnn8.2
TensorRT 8.2.0.6	10.2	8.2	/fs00/software/tensorrt/8.2.0.6-cuda11.4-cudnn8.2	tensorrt/8.2.0.6-cuda10.2-cudnn8.2



# AMD

## AMD Optimizing C/C++ Compiler

Name	Path	Module
AMD Optimizing C/C++ Compiler 2.3.0 (AOCC)	/fs00/software/aocc/2.3.0	aocc/2.3.0
AMD Optimizing C/C++ Compiler 2.1.0 (AOCC)	/fs00/software/aocc/2.1.0	aocc/2.1.0
AMD Optimizing C/C++ Compiler 2.0.0 (AOCC)	/fs00/software/aocc/2.0.0	aocc/2.0.0

## AMD Optimizing CPU Libraries

Name	Path	Module
AMD Optimizing CPU Libraries 2.2 (AOCL)	/fs00/software/aocl/2.2	aocl/2.2
AMD Optimizing CPU Libraries 2.0 (AOCL)	/fs00/software/aocl/2.0	aocl/2.0

# Python

License

## Anaconda

Name	Path	Module
Anaconda 3 (Python3) Latest	/fs00/software/anaconda/3	anaconda/3
Anaconda 2 (Python2) Latest	/fs00/software/anaconda/2	anaconda/2
Anaconda 5.0.1 (Python 3.6)	/fs00/software/anaconda/3-5.0.1	anaconda/3-5.0.1
Anaconda 5.0.1 (Python 2.7)	/fs00/software/anaconda/2-5.0.1	anaconda/2-5.0.1
Anaconda 3.4.1 (Python 3.6)	/fs00/software/anaconda/3-3.4.1	anaconda/3-3.4.1
Anaconda 3.4.1 (Python 2.7)	/fs00/software/anaconda/2-3.4.1	anaconda/2-3.4.1

# Golang

## Golang

Name	Path	Module
Golang 1.21.6	/fs00/software/golang/1.21.6	golang/1.21.6
Golang 1.19.5	/fs00/software/golang/1.19.5	golang/1.19.5
Golang 1.18.10	/fs00/software/golang/1.18.7	golang/1.18.10
Golang 1.17.13	/fs00/software/golang/1.17.13	golang/1.17.13
Golang 1.16.15	/fs00/software/golang/1.16.15	golang/1.16.15
Golang 1.15.15	/fs00/software/golang/1.15.15	golang/1.15.15

# Open MPI

## Open MPI

Name	Compiler	Path	Module
Open MPI 4.1.2	GNU Compiler Collection (GCC) 11.2.0	/fs00/software/openmpi/4.1.2-gcc11.2.0	openmpi/4.1.2-gcc11.2.0
Open MPI 3.1.2	GNU Compiler Collection (GCC) 8.2.0	/fs00/software/openmpi/3.1.2-gcc8.2.0	openmpi/3.1.2-gcc8.2.0
Open MPI 1.10.0	Intel C++ Compiler XE 15.0 Update 3 & Fortran Compiler XE 15.0 Update 3	/fs00/software/openmpi/1.10.0-iccifort-15.0.3	openmpi/1.10.0-iccifort-15.0.3
Open MPI 1.10.0	GNU Compiler Collection (GCC) 5.2.0	/fs00/software/openmpi/1.10.0-gcc-5.2.0	openmpi/1.10.0-gcc-5.2.0
Open MPI 1.10.5	GNU Compiler Collection (GCC) 5.4.0	/fs00/software/openmpi/1.10.5-gcc5.4.0	openmpi/1.10.5-gcc5.4.0

# Tcl/TK

## Tcl/Tk

Name	Compiler	Path	Module
Tcl/Tk 8.6.12	GNU Compiler Collection (GCC) 11.2.0	/fs00/software/tcl/8.6.12-gcc11.2.0	tcl/8.6.12-gcc11.2.0
Tcl/Tk 8.6.6	Intel Parallel Studio XE 2017 Update 2	/fs00/software/tcl/8.6.6-ips2017u2	tcl/8.6.6-ips2017u2
Tcl/Tk 8.6.4		/fs00/software/tcl/8.6.4	tcl/8.6.4
Tcl/Tk 8.6.4	Intel Parallel Studio XE 2016 Update 2	/fs00/software/tcl/8.6.4-ips2016u2	tcl/8.6.4-ips2016u2
Tcl/Tk 8.6.4	Intel Parallel Studio XE 2016 Update 2	/fs00/software/tcl/8.6.4-ips2016u2-avx2	tcl/8.6.4-ips2016u2-avx2

?????

□□□□□□

**License**□□□□□□□□

## FFTW 3.3.7

/fs00/software/fftw/3.3.7-iccifort-17.0.6-\* □□ iccifort/17.0.6

## FFTW 3.3.8

/fs00/software/fftw/3.3.8-ips2019u5 □□ ips/2019u5

## LAMMPS 11Aug17

/fs00/software/lammps/11Aug17

## OpenFOAM® v1806

/fs00/software/openfoam/v1806-ips2017u6

source /fs00/software/openfoam/v1806-ips2017u6/OpenFOAM-v1806/etc/bashrc

## P4vasp 0.3.29

/fs00/software/p4vasp/0.3.29

Modulefile: p4vasp/0.3.29

## Phonopy 1.11.2

/fs00/software/phonopy/1.11.2

## Quantum ESPRESSO 5.2.0 & 6.1

/fs00/software/qe/5.2.0-ips2015u3/ □□ ips/2015u3

/fs00/software/qe/6.1-ips2017u2/ □□ ips/2017u2

# ShengBTE

/fs00/software/shengbte □□ iccifort/15.0.3 openmpi/1.10.0-iccifort-15.0.3

# Siesta 3.2-pl-5

/fs00/software/siesta/3.2-pl-5 □□ ips/2017u6

# thirdorder 1.0.2 04d3f46feb78

/fs00/software/thirdorder/1.0.2

Modulefile: thirdorder/1.0.2 □□ anaconda/2-4.3.1 spglib/1.9.9

# TBPLaS

/fs00/software/tbplas

# MKL+MPI Version

Modulefile:









- oneapi/2024.0/compiler/2024.0.2
- oneapi/2024.0/fort/2024.0.2
- oneapi/2024.0/mkl/2024.0
- oneapi/2024.0/mpi/2021.11

# VASP6 GPU?N??

[illegible]

[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 

11 NVIDIA HPC-SDK 20.9

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

```

tarball
├── wget
│   └── version >=10.0
├── nvidia-smi
└── cuda
  
```

☐ HPC-SDK 20.9 ☐ /usr/software/nv-hpcsdk

```
export NVARCH=`uname -s`_`uname -m`;
export NVCOMPILERS=/usr/software/nv-hpcsdk #XXXXXXXXXX
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#####  
##### intel##### mpirun#####

bashrc#####

bashrc

????

##### NVIDIA HPC-SDK 20.9#####  
NCCL, ##### FFTW, ##### HPC-SDK#####

CUDA Toolkit, QD,

##### FFTW##### nvhpc-sdk#####  
GNU##### intel

hpc-sdk#####

#####

##### /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_dbdbuf \
-D_OPENACC \
-DUSENCCL -DUSENCCLP2P
```

```
CPP      = nvfortran -Mpreprocess -Mfree -Mextend -E $(CPP_OPTIONS) *$(FUFFIX) >
*$(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 -00 -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 precision
QD          = $(NVR00T)/compilers/extras/qd          #□□□□□□□□
LLIBS       += -L$(QD)/lib -lqdm -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
```

???????

1. nccl openacc gpu .

2.INCAR NCORE openacc 1.

3.INCAR NSIM KPAR KPAR  
 GPU NSIM cpu .

GPU

VASP

# Quantum Espresso

## ??Apptainer

qe7.1 Fe0\_test.in 1 GPU 723090ib pw.x

```
#BSUB -J Fe0_test
#BSUB -q 723090ib
#BSUB -gpu num=1

export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
QE="apptainer run --nv /fs00/software/singularity-images/ngc_quantum_espresso_qe-7.1.sif"
${QE} pw.x < Fe0_test.in > Fe0_test.out
```

# NAMD

## NAMD 2.12 (2016-12-22)

- /fs00/software/namd/2.12

■■■■■■■■■■

in.conf■■■

48■■■■

e5v3ib■■

```
#BSUB -n 48
#BSUB -q e5v3ib

input=in.conf
#bindir=/fs00/software/namd/2.12/verbs/
bindir=/fs00/software/namd/2.12/ibverbs/

nodefile=nodelist
echo "group main" > $nodefile
for i in `echo $LSB_HOSTS`
do
    echo "host $i" >> $nodefile
done

${bindir}charmrun ++remote-shell ssh ++nodelist $nodefile +p$LSB_DJOB_NUMPROC ${bindir}namd2
$input
```

# OOMMF

## The Object Oriented MicroMagnetic Framework (OOMMF) 1.2 alpha 6

- /fs00/software/oommf/12a6-tcl8.6.4-ips2016u2 ☐ tcl/8.6.4-ips2016u2 ☐ ips/2016u2
- /fs00/software/oommf/12a6-tcl8.6.4-ips2016u2-avx2 ☐ tcl/8.6.4-ips2016u2-avx2 ☐ ips/2016u2

☐☐☐☐☐☐☐☐☐☐☐☐

sample.mif☐☐☐☐

72☐☐☐☐☐

6140ib☐☐

```
#BSUB -q 6140ib
#BSUB -n 72

module load ips/2016u2
module load tcl/8.6.4-ips2016u2-avx2

oommfin=sample.mif

oommfrun=/fs00/software/oommf/12a6-tcl8.6.4-ips2016u2-avx2/oommf.tcl

OOMMF_HOSTPORT=`tclsh $oommfrun launchhost 0`
export OOMMF_HOSTPORT
tclsh $oommfrun mmArchive
tclsh $oommfrun boxsi -numanodes auto -threads $LSB_DJOB_NUMPROC $oommfin
tclsh $oommfrun killoommf all
```

# Mumax3

## mumax 3.10

- /fs00/software/mumax/3.10-cuda11.0/

■■■■■■■■■■

sample.mx3■■■ 1■ GPU■■■ 723090ib■■

```
#BSUB -q 723090ib
#BSUB -gpu num=1

mx3in=sample.mx3

module load cuda/11.2.0
/fs00/software/mumax/3.10-cuda11.0/mumax3 $mx3in
```



?????

■■■■■■■

License■■■■■■■■■

## AWS CLI v2

Name	Path	Module
AWS CLI current	/fs00/software/aws-cli/v2/current	aws-cli/current
AWS CLI 2.9.6	/fs00/software/aws-cli/v2/2.9.6	aws-cli/2.9.6

## bbcp

Name	Path	Module
bbcp 14.04.14.00.1	/fs00/software/bbcp/14.04.14.00.1	bbcp/14.04.14.00.1

## Boost

Name	Path	Module
Boost 1.72.0	/fs00/software/boost/1.72.0	boost/1.72.0
Boost 1.58.0	/fs00/software/boost/1.58.0	boost/1.58.0

## CMake

Name	Path	Module
CMake 3.23.2	/fs00/software/cmake/3.23.2/	cmake/3.23.2
CMake 3.16.3	/fs00/software/cmake/3.16.3/	cmake/3.16.3
CMake 3.11.4	/fs00/software/cmake/3.11.4/	cmake/3.11.4

## Git

Name	Path	Module
Git 2.38.1	/fs00/software/git/2.38.1	git/2.38.1

# Grace

Name	Path	Module
Grace 5.1.25	/fs00/software/grace/5.1.25	grace/5.1.25

# HDF5

Name	Path	Module
HDF5 1.10.5	/fs00/software/hdf5/1.10.5	hdf5/1.10.5

# libpng

Name	Path	Module
libpng 1.5.26	/fs00/software/libpng/1.5.26	libpng/1.5.26

# jq

Name	Path	Module
jq 1.7	/fs00/software/jq/1.7	jq/1.7

# Libxc

Name	Compiler	Path	Module
Libxc 5.2.2	GNU Compiler Collection (GCC) 11.2.0	/fs00/software/libxc/5.2.2	libxc/5.2.2

# libzip

Name	Path	Module
libzip 1.6.1	/fs00/software/libzip/1.6.1	libzip/1.6.1

# NetCDF-C

Name	Path	Module
NetCDF-C 4.7.0	/fs00/software/netcdf/c-4.7.0	netcdf/c-4.7.0

# PCRE

Name	Path	Module
PCRE 8.39	/fs00/software/pcre/8.39	pcre/8.39

# Qt

Name	Path	Module
Qt 5.11.1	/fs00/software/qt/5.11.1	qt/5.11.1

# rclone

Name	Path	Module
rclone latest	/fs00/software/rclone/latest	rclone/latest
rclone 1.66.0	/fs00/software/rclone/1.66.0	rclone/1.66.0

# Spglib (OpenMP)

Name	Compiler	Path	Module
Spglib 1.9.9		/fs00/software/spglib/1.9.9	spglib/1.9.9
Spglib 1.9.0	GNU Compiler Collection (GCC) 5.2.0	/fs00/software/spglib/1.9.0-gcc5.2.0	spglib/1.9.0-gcc5.2.0

# tmux

Name	Path	Module
tmux 3.3a	/fs00/software/tmux/3.3a	tmux/3.3a

# zlib

Name	Path	Module
zlib 1.2.11	/fs00/software/zlib/1.2.11	zlib/1.2.11

# Singularity Image

/fs00/software/singularity-images/



# gnuplot

## gnuplot

Name	Path	Module
gnuplot 5.2.7	/fs00/software/gnuplot/5.2.7	gnuplot/5.2.7
gnuplot 5.2.2	/fs00/software/gnuplot/5.2.2	gnuplot/5.2.2
gnuplot 5.0.6	/fs00/software/gnuplot/5.0.6	gnuplot/5.0.6
gnuplot 5.0.1	/fs00/software/gnuplot/5.0.1	gnuplot/5.0.1

# OVITO

## OVITO

Name	Path	Module
OVITO 3.7.12	/fs00/software/ovito/3.7.12	ovito/3.7.12
OVITO 2.9.0	/fs00/software/ovito/2.9.0	ovito/2.9.0

# Vim

## Vim

Name	Path	Module
Vim 9.0.1677	/fs00/software/vim/9.0.1677	vim/9.0.1677
Vim 8.2.0488	/fs00/software/vim/8.2.0488	vim/8.2.0488
Vim 8.1	/fs00/software/vim/8.1	vim/8.1

# Zsh

Name	Path	Module
Zsh latest	/fs00/software/zsh/latest	zsh/latest
Zsh 5.8	/fs00/software/zsh/5.8	zsh/5.8

# Environment Modules

Environment Modules ▢ Zsh

```
echo "source /fs00/software/modules/latest/init/profile.sh" >> ~/.zshrc
```

??????

-   Zsh  \$  Bash  Shell

```
module load zsh/latest && exec zsh
```

- [illegible]

# Oh My Zsh

??

```
git clone https://mirror.nju.edu.cn/git/ohmyzsh.git
cd ohmyzsh/tools
REMOTE=https://mirror.nju.edu.cn/git/ohmyzsh.git sh install.sh
```

???? Oh My Zsh ???? ?

```
git -C $ZSH remote set-url origin https://mirror.nju.edu.cn/git/ohmyzsh.git
git -C $ZSH pull
```



??

omz update

??

# Powerlevel10k

??

```
git clone --depth=1 https://mirror.nju.edu.cn/git/powerlevel10k.git ${ZSH_CUSTOM:-$HOME/.oh-my-zsh/custom}/themes/powerlevel10k
```

```
~/.zshrc ZSH_THEME="powerlevel10k/powerlevel10k"
```

??

```
cd ${ZSH_CUSTOM:-$HOME/.oh-my-zsh/custom}/themes/powerlevel10k && git pull
```

256???

[illegible]

```
echo "export TERM=xterm-256color" >> ~/.zshrc
```

????????

~/.p10k.zsh

1. `POWERLEVEL9K_RIGHT_PROMPT_ELEMENTS` `context` `POWERLEVEL9K_LEFT_PROMPT_ELEMENTS`
2. `typeset -g POWERLEVEL9K_CONTEXT_{DEFAULT,SUDO}_{CONTENT,VISUAL_IDENTIFIER}_EXPANSION=`
3. `typeset -g POWERLEVEL9K_CONTEXT_PREFIX=` `'`

??

## zsh-autosuggestions

??

```
git clone https://mirror.nju.edu.cn/git/zsh-autosuggestions ${ZSH_CUSTOM:-~/.oh-my-zsh/custom}/plugins/zsh-autosuggestions
```

❏ ~/.zshrc ❏ plugins= ❏❏ zsh-syntax-highlighting

```
plugins=( ... zsh-autosuggestions)
```

??

```
cd ${ZSH_CUSTOM:- ~/.oh-my-zsh/custom}/plugins/zsh-autosuggestions && git pull
```

## zsh-syntax-highlighting

??

```
git clone https://mirror.nju.edu.cn/git/zsh-syntax-highlighting.git ${ZSH_CUSTOM:- ~/.oh-my-zsh/custom}/plugins/zsh-syntax-highlighting
```

❏ ~/.zshrc ❏ plugins= ❏❏❏ zsh-syntax-highlighting

```
plugins=( [plugins...] zsh-syntax-highlighting)
```

??

```
cd ${ZSH_CUSTOM:- ~/.oh-my-zsh/custom}/plugins/zsh-syntax-highlighting && git pull
```

# AlphaFold 2

/fs00/software/alphafold/2.3.2/AlphaFold-v2.3.2.sif

```
#BSUB -J alphafold
#BSUB -q gpu
#BSUB -n 16
#BSUB -gpu num=1

export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
export MKL_NUM_THREADS="$LSB_DJOB_NUMPROC"

ALPHAFOLD_DATADIR=/fsb/data/alphafold/2
ALPHAFOLD_IMAGE=AlphaFold-v2.3.2.sif

ALPHAFOLD_APP=/app/alphafold

RUN_ALPHAFOLD="apptainer run --bind ${ALPHAFOLD_DATADIR}:${ALPHAFOLD_APP}/download \
    --nv ${ALPHAFOLD_IMAGE}"

${RUN_ALPHAFOLD} python ${ALPHAFOLD_APP}/run_alphafold.py --use_gpu_relax \
    --data_dir=${ALPHAFOLD_APP}/download \
    --uniref90_database_path=${ALPHAFOLD_APP}/download/uniref90/uniref90.fasta \
    --mgnify_database_path=${ALPHAFOLD_APP}/download/mgnify/mgy_clusters_2022_05.fa \
    --
bfd_database_path=${ALPHAFOLD_APP}/download/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.
sorted_opt \
    --pdb70_database_path=${ALPHAFOLD_APP}/download/pdb70/pdb70 \
    --uniref30_database_path=${ALPHAFOLD_APP}/download/uniref30/UniRef30_2021_03 \
    --template_mmcif_dir=${ALPHAFOLD_APP}/download/pdb_mmcif/mmcif_files \
    --obsolete_pdbs_path=${ALPHAFOLD_APP}/download/pdb_mmcif/obsolete.dat \
    --model_preset=monomer \
    --max_template_date=2022-10-1 \
    --db_preset=full_dbs \
    --output_dir=output \
    --fasta_paths=input/input.fasta
```

# AlphaFold 3

/fs00/software/alphafold/3.0.0/AlphaFold-v3.0.0.sif

## 0. ????

alphafold3 Google DeepMind json

- data pipeline:  
(multi-sequence alignment, msa) (templates)  
json
- inference: msa templates json mmCIF  
confidence score

github apptainer alphafold3  
term of use  
Google DeepMind

## 1. ????

```
path_to_af3db="/fsb/data/alphafold/3"
path_to_af3container="/fs00/software/alphafold/3.0.0/AlphaFold-v3.0.0.sif "

io_dir=</path/to/your/input/and/output>
weights_dir=<path/to/directory/containing/your/af3-weights>

RUN_ALPHAfold="apptainer run --nv --bind
${path_to_af3db}:/databases,${io_dir}:/host_iopath,${weights_dir}:/af3_weights
${path_to_af3container} python run_alphafold.py"
```

alphafold3  
run\_alphafold.py github  
( )

```
${RUN_ALPHAFAOLD} --help
```

```
input.json ${io_dir} alphafold3
```

```
${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
--json_path=/host_iopath/input.json --output_dir=/host_iopath/
```

```
input.json name ${io_dir} data pipeline json
confidence score log stderr (
python logging ) input documentation output documentation
```

## 2. data pipeline?inference

```
data pipeline inference data pipeline cpu
gpu gpu gpu
cpu data pipeline ( json) gpu
```

```
bool --run_data_pipeline --run_inference
True.
```

```
:
```

- data pipeline (cpu job)

```
${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
--json_path=/host_iopath/input.json --output_dir=/host_iopath/ \
--run_inference=False
```

- inference (gpu job)

```
${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
--json_path=/host_iopath/input.json --output_dir=/host_iopath/ \
--run_data_pipeline=False
```

```
msa templates
alphafold3 msa templates json --
run_data_pipeline=False msa templates json
DeepMind-input documentation msa templates json
mb
```

## 3.

run\_alphafold.py

`{RUN_ALPHAFOLD} --help`

run\_alphafold.py

3

- `--input_dir` `--json_path` `input_dir`  
`input_dir` `json`
- `--jackhmmer_n_cpu` `--nhmmer_n_cpu` `cpu cores`
- `random seed` `alphafold3` `random seed`  
`input.json`

4.

data pipeline inference gpu

- 2PV7 homomer 298
- 1AKE homomer 214

83a100ib 734090d A100 (memory 40 G) 4090d  
(memory 24 G) inference. 722080tiib 72rtxib . GPU  
[performance documentation](#) alphafold3 A100(80G),  
A100(40 G) H100 4090

data pipeline inference

- 8 cpu cores 300 msa templates 1.5-2 h  
msa templates 10 s
- alphafold3 5  
100 s inference

performance [performance documentation](#)

5.

2PV7 RMSD=4.410 ( : Angstrom )  
A:B - A:B RMSD 4 RMSD 3.012, 2.759, 2.971,  
2.740. alphafold3 alphafold2. 2 subunits DockQ  
0.499>0.23 docking

1AKE 1AKE RMSD=18.176 4AKE RMSD=26.791  
alphafold2-multimer subunits DockQ=0.019<<0.23  
Alphafold3 4090d  
A100

“ dockQ (Mirabello & Wallner, 2024, Bioinformatics) subunits  
0-1 <0.23 >0.8



```
/fs00/software/rosettafold/1.1.0
```

```
#BSUB -J RoseTTAFold
```

```
#BSUB -q gpu
```

```
#BSUB -n 8
```

```
#BSUB -gpu num=1
```

```
##### Configurie Numpy threads #####
```

```
export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
```

```
export MKL_NUM_THREADS="$LSB_DJOB_NUMPROC"
```

```
##### Definition #####
```

```
ROSETTAFOLD_DATADIR=/fsb/data/rosettafold      # path to RosettaFold data (host)
ROSETTAFOLD_IMAGE=RosettaFold-1.1.0.sif        # path to RosettaFold image (host)
ROSETTAFOLD_APPDIR=/app/RosettaFold            # path to RosettaFold working directory
(container)
```

```
##### Database #####
```

UNIREF30 DB=\$ROSETTAFOLD DATADIR/UniRef30 2020 06

BFD\_DB=\$ROSETTAFOLD\_DATADIR/bfd

PDB100 DB=\$ROSETTAFOLD DATADIR/pdb100\_2021Mar03

### ##### Example #####

```
RUN_ROSETTAFOLD="apptainer run --bind $UNIREF30_DB:$ROSETTAFOLD_APPDIR/UniRef30_2020_06 \
--bind $BFD_DB:$ROSETTAFOLD_APPDIR/bfd \
--bind $PDB100_DB:$ROSETTAFOLD_APPDIR/pdb100_2021Mar03 \
--nv $ROSETTAFOLD IMAGE"
```

```
# For monomer structure prediction (e2e)
```



```
${RUN_ROSETTAFOLD} $ROSETTAFOLD_APPDIR/run_e2e_ver.sh $ROSETTAFOLD_APPDIR/example/input.fa  
output/
```

```
# For monomer structure prediction (pyrosetta)
```

```
${RUN_ROSETTAFOLD} $ROSETTAFOLD_APPDIR/run_pyrosetta_ver.sh  
$ROSETTAFOLD_APPDIR/example/input.fa output/
```

```
# For complex modeling
```

```
${RUN_ROSETTAFOLD} python $ROSETTAFOLD_APPDIR/network/predict_complex.py \  
    -i $ROSETTAFOLD_APPDIR/example/complex_modeling/paired.a3m \  
    -o output/ -Ls 218 310
```

```
# For PPI screening using faster 2-track version (example input and output are at  
example/complex_2track)
```

```
${RUN_ROSETTAFOLD} python $ROSETTAFOLD_APPDIR/network_2track/predict_msa.py \  
    -msa $ROSETTAFOLD_APPDIR/example/complex_2track/input.a3m \  
    -npz output/complex.npz -L1 218
```

# ParallelFold 2

```
/fs00/software/parallelfold/2.0-2.3.1/ParallelFold-v2.0-with-AlphaFold-v2.3.1.sif
```

```
#BSUB -J parafold
#BSUB -q gpu
#BSUB -n 16
#BSUB -gpu num=1

export OMP_NUM_THREADS="${LSB_DJOB_NUMPROC}"
export MKL_NUM_THREADS="${LSB_DJOB_NUMPROC}"

ALPHAFOLD_DATADIR=/fsb/data/alphafold/2
PARAFOLD_IMAGE=ParallelFold-v2.0-with-AlphaFold-v2.3.1.sif

PARAFOLD_APP=/app/ParallelFold

RUN_PARAFOLD="apptainer run --bind ${ALPHAFOLD_DATADIR}:${PARAFOLD_APP}/download \
    --nv ${PARAFOLD_IMAGE}"

${RUN_PARAFOLD} python ${PARAFOLD_APP}/run_alphafold.py --use_gpu_relax \
    --parameter_path=${PARAFOLD_APP}/download/params \
    --uniref90_database_path=${PARAFOLD_APP}/download/uniref90/uniref90.fasta \
    --mgnify_database_path=${PARAFOLD_APP}/download/mgnify/mgy_clusters_2022_05.fa \
    --
bfd_database_path=${PARAFOLD_APP}/download/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_opt \
    --pdb70_database_path=${PARAFOLD_APP}/download/pdb70/pdb70 \
    --uniref30_database_path=${PARAFOLD_APP}/download/uniref30/UniRef30_2021_03 \
    --template_mmcif_dir=${PARAFOLD_APP}/download/pdb_mmcif/mmcif_files \
    --obsolete_pdbs_path=${PARAFOLD_APP}/download/pdb_mmcif/obsolete.dat \
    --model_preset=monomer \
    --max_template_date=2022-10-1 \
    --db_preset=full_dbs \
    --output_dir=output \
    --fasta_paths=${PARAFOLD_APP}/input/input.fasta
```