



- [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

Name	Compiler	Path	Module
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

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

Name	CUDA	Path	Module
cuDNN v7.6.5.32	10.2	/fs00/software/cudnn/10.2-v7.6.5.32	cudnn/10.2-v7.6.5.32
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
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

VASP6 GPU N

()

vasp vasp gpu openacc cuda
vasp6.2 openacc

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

NVIDIA HPC-SDK 20.9

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

wget tarball
nvidia-smi cuda
version >=10.0

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#####
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 \  
-Dfock_dblbuf \  
-D_OPENACC \  
-DUSENCCL -DUSENCCLP2P
```

```
CPP      = nvfortran -Mpreprocess -Mfree -Mextend -E $(CPP_OPTIONS) *$(FUUFFIX) > *$(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 NVROOT automatically
```

```
NVROOT    =$(shell which nvfortran | awk -F /compilers/bin/nvfortran '{ print $$1 }')
```

```
#or set NVROOT manually
```

```
#NVHPC     ?= /opt/nvidia/hpc_sdk
```

```
#NVVERSION = 20.9
```

```
#NVROOT    = $(NVHPC)/Linux_x86_64/$(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      = $(NVROOT)/compilers/extras/qd      #[]
LLIBS    += -L$(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 O1 and O2 objects
SOURCE_O1 := pade_fit.o
SOURCE_O2 := 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
GPU
make gpu
vasp_std
```



```
1. nccl openacc gpu .
```

```
2.INCAR NCORE openacc 1.
```














```
3.INCAR NSIM KPAR
GPU NSIM cpu KPAR
.
```

```
GPU
```

```
VASP_
```

Quantum Espresso

Apptainer

  qe7.1     FeO_test.in   1  GPU   723090ib   pw.x

```
#BSUB -J FeO_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 < FeO_test.in > FeO_test.out
```

NAMD

NAMD 2.12 (2016-12-22)

- /fs00/software/namd/2.12

XXXXXXXXXX

in.confXXXX

48XXXXXX

e5v3ibXX

```
#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 [\[1\]](#) tcl/8.6.4-ips2016u2 [\[2\]](#) ips/2016u2
- /fs00/software/oommf/12a6-tcl8.6.4-ips2016u2-avx2 [\[1\]](#) tcl/8.6.4-ips2016u2-avx2 [\[2\]](#) 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

The diagrams show three ways to represent the number 10 as a sum of 2s:

- Two vertical rectangles, each divided into two equal halves, representing $2 + 2$.
- Three vertical rectangles, each divided into two equal halves, representing $2 + 2 + 2$.
- Five vertical rectangles, each divided into two equal halves, representing $2 + 2 + 2 + 2 + 2$.

Environment Modules

Environment Modules ▮ Zsh

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

--	--	--	--	--	--

- \$ Bash Shell

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

- Zsh PS1\$ Shell Zsh Zsh

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
```



```
ZSH_THEME="powerlevel10k/powerlevel10k"
```



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

256 xterm ☐☐☐[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=/bbfs/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=${ALPHAFOLD_APP}/download/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_o
pt \
    --pdb70_database_path=${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

The diagram consists of two horizontal rows of small rectangular boxes. The top row contains 28 boxes, and the bottom row contains 20 boxes. Above the first box of the top row is the label 'alphafold3'. Above the first four boxes of the top row is the label 'Google DeepMind'. To the right of the top row, aligned with its end, is the label 'json'. The boxes themselves are empty and have thin black outlines.

- data pipeline:

```
graph LR; Input[ ] --> MSAlign[multi-sequence alignment, msa]; MSAlign --> Templates[ ]; Templates --> JSON[json]; JSON --> Inference[inference]; Inference --> ConfScore[confidence score];
```
- inference:

github apptainer alphafold3

Google DeepMind

term of use

1.

--	--	--	--

```
path_to_af3db="/bbfs/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"
```

[illegible]

$$\left(\begin{array}{c} \square \\ \square \\ \square \\ \square \\ \square \end{array} \right) \quad \left(\begin{array}{c} \square \\ \square \\ \square \\ \square \\ \square \end{array} \right)$$

```

${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
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  msa  templates  json
Mb

```

3.

```
run_alphafold.py --input_dir input_dir --json_path input_dir --jackhmmer_n_cpu 3 --nhmmer_n_cpu 3 --random_seed random_seed --input.json input.json
```

- --input_dir input_dir --json_path input_dir --input_dir input_dir --json_path input_dir
- --jackhmmer_n_cpu 3 --nhmmer_n_cpu 3 --cpu_cores 3
- --random_seed random_seed --alphafold3_random_seed random_seed --input.json input.json

4. Performance

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. Results

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

RoseTTAFold

/fs00/software/rosettafold/1.1.0

apptainer bind home RoseTTAFold folding conda
--no-home

```
#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=/bbfs/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.fasta  
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=/bbfs/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=${PARAFOLD_APP}/download/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_op
t \
    --pdb70_database_path=${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
```