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- /fs00/software
- /fs00/software/singularity-images/

□□□

- 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

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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

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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

LAMMPS 23Jun2022

/fs00/software/lammps/23Jun2022

LAMMPS 22Jul2025

/fs00/software/lammps/22Jul2025

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/ifort/2024.0.2
- oneapi/2024.0/mkl/2024.0
- oneapi/2024.0/mpi/2021.11

VASP6 GPU □□

VASP6 GPU□ N□□ □□□□

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□□ vasp□□□□□□□□□□ vasp gpu□□□□□□□ openacc□□□□□□□□□ cuda □□□□□□□□□□□□□□ vasp6.2 □ openacc□□□□□□□□□□□□□□ □□□□□□

```
https://www.vasp.at/wiki/index.php/OpenACC_GPU_port_of_VASP
```

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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
```

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□□ 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□□□□□□□□□□□□□□□□□

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

□□ FFTW□□□□□□ nvhpc-sdk□□□□□□□□□□□□□□□□□□□□□□ hpc-sdk□□□□□□□□□ GNU□□ intel □□□□□□□□□□□□□□□□□□□□

```
          -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) $*$(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 -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 precsion
QD         = $(NVROOT)/compilers/extras/qd                    #□□□□□□□□
LLIBS      += -L$(QD)/lib -lqdmod -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    = fftmpiw.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
```

□□□□□□□□□□

```
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□□□□□□□□□□□□□□ `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

□□□□□□□□□□□□□ 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

mumax3 □□	□□□□	□□□□□ **CUDA** □□	□□□□□□□ **GLIBC □□**	□□□□□□
3.10-cuda11.0	`/fs00/software/mumax/3.10-cuda11.0`	`cuda/11.2.0`	`GLIBC_2.4`	□□□□□□ CentOS 7 □
3.11.1-cuda12.3	`/fs00/software/mumax/3.11.1-cuda12.3`	`cuda/12.3.1`	`GLIBC_2.3.2`	□ **Rocky 9** □□□□□□□□ Rocky 9 □□□□
3.11.1-cuda12.8	`/fs00/software/mumax/3.11.1-cuda12.8`	`cuda/12.8.1-el9`	`GLIBC_2.34`	□□ □ Rocky 9 / RHEL 9 □□□□□□□

□□□□□□ `module load cuda/<□□□>` □

□□□□□□□□□□□□□□ 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
```

□□□□□ CUDA 12 □□□□□□ Rocky 9□□□□□

□□□□□□□□□□□□□□□□□□□□□ `mumax3-convert`□ `mumax3-plot`□

□□□□

□□□□□□□□ **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 6.0.5-el9	/fs00/software/gnuplot/6.0.5-el9	gnuplot/6.0.5-el9	□ qt □□□□□□□□□□□□□□□□
gnuplot 6.0.4-el9-gui	/fs00/software/gnuplot/6.0.4-el9	gnuplot/6.0.4-el9-gui	□ qt5 □□□□□□□□□□□□□□□□
gnuplot 5.2.7	/fs00/software/gnuplot/5.2.7	gnuplot/5.2.7	□ qt4 □□□□□□□□□□□□□□□□
gnuplot 5.2.2	/fs00/software/gnuplot/5.2.2	gnuplot/5.2.2	□ qt □□□□□□□□□□□□□□□□
gnuplot 5.0.6	/fs00/software/gnuplot/5.0.6	gnuplot/5.0.6	□ qt □□□□□□□□□□□□□□□□
gnuplot 5.0.1	/fs00/software/gnuplot/5.0.1	gnuplot/5.0.1	□ X11/qt □□□□□□□□□□□□□□□□

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
```

□□□□□

- □□□□□□□□□□□□□□□□ `$` □□□□□□□ Bash □□□ Shell □□□□□□□□□□□□□ Zsh

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

- □□□ Zsh □□□ Shell □□□□□□□□□ Zsh□□□□□ Zsh □□□□□□□□□□□□ PS1□□ `$` □□□ $+□□□□□□□□□□□□

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□□□

□□ xterm □□□ 256□□□□□□□□□□□

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

□□□□□□□□□

□□□□□□□□□□□

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□□□

```
${RUN_ALPHAFOLD} --help
```

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

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

- inference (gpu job)

  ```
  ${RUN_ALPHAFOLD} --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} --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□□□□□

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=/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=${PARAFOLD_APP}/download/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.s
orted_opt \
    --pdb70_database_path=${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
```