

Center for Theoretical Physics of Complex Systems

Fermi Cluster system

- Application installed list.
 - Environment module list.
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- Refer to the contents when using module
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1. Use the "module help" command.

Ex.

```
[root@fermi ~]# module help meep/intel-18.0.3/1.7.0

----- Module Specific Help for 'meep/intel-18.0.3/1.7.0' -----

* meep-1.7.0 with intel-18.0.3
* Using the GMP-6.1.2 library.
* Using the guile-2.2.4 library compiled with gcc-4.8.5.
* Using the HDF5-1.10.4 library compiled with intel-18.0.3.
* Using the FFTW-3.3.8 library compiled with intel-18.0.3.
* Using the libctl-4.2.0 library compiled with intel-18.0.3.
* Using the openmpi-2.1.5 version MPI compiled with intel-18.0.3.
* How to use dependency package modulefiles load.

    module load intel/18.0.3
    module load gmp/6.1.2
    module load guile/gcc-4.8.5/2.2.4
    module load hdf5/intel-18.0.3/1.10.4
    module load fftw/intel-18.0.3/3.3.8/double
    module load libctl/intel-18.0.3/4.2.0
    module load intel-18.0.3/openmpi/2.1.5

* Autoloading dependency packages.

[root@fermi ~]#
```

2. Use the "module purge" command to avoid library conflicts.

Application & Library	Binary File & Directory Path	Version	module purge	Remarks
SGE	/opt/sge/bin/lx-amd64/qstat /opt/sge/bin/lx-amd64/qhost /opt/sge/bin/lx-amd64/qsub /opt/sge/bin/lx-amd64/qdel	8.1.8	OS default environment.	
Intel Compiler	/opt/intel/2017up1	17.0.1	module load intel/17.0.1	
	/opt/intel/2018up3	18.0.3	module load intel/18.0.3	
GCC	/usr/bin/gcc /usr/bin/g++ /usr/bin/gfortran	4.8.5	OS default environment.	
	/opt/gcc/7.3.0/bin/gcc /opt/gcc/7.3.0/bin/g++ /opt/gcc/7.3.0/bin/gfortran	7.3.0	module load gcc/7.3.0	
	/opt/gcc/8.2.0/bin/gcc /opt/gcc/8.2.0/bin/g++ /opt/gcc/8.2.0/bin/gfortran	8.2.0	module load gcc/8.2.0	
	/opt/gcc/9.2.0/bin/gcc /opt/gcc/9.2.0/bin/g++ /opt/gcc/9.2.0/bin/gfortran	9.2.0	module load gcc/9.2.0	
Intel MPI	/opt/intel/2017up1/ compilers_and_libraries_2017.1.132/linux/mpi/intel64/bin /mpirun	2017.1.1 32	module load intel/17.0.1	
	/opt/intel/2018up3/ compilers_and_libraries_2018.3.222/linux/mpi/intel64/bin /mpirun	2018.3.2 22	module load intel/18.0.3	
OpenMPI	/opt/mpi/intel-17.0.1/openmpi-2.1.5/bin/mpirun	2.1.5	module load intel/17.0.1 module load intel-17.0.1/openmpi/2.1.5	• OpenMPI with Intel Compiler 17.0.1 • Autoloading dependency packages.
	/opt/mpi/intel-18.0.3/openmpi-2.1.5/bin/mpirun		module load intel/18.0.3 module load intel-18.0.3/openmpi/2.1.5	• OpenMPI with Intel Compiler 18.0.3 • Autoloading dependency packages.
	/opt/mpi/gcc-4.8.5/openmpi-2.1.5/bin/mpirun		module load gcc-4.8.5/openmpi/2.1.5	• OpenMPI with GCC 4.8.5

Mvapich2	/opt/mpi/intel-17.0.1/mvapich2-2.3/bin/mpirun	2.3	module load intel/17.0.1 module load intel-17.0.1/mvapich2/2.2	• Mvapich2 with Intel Compiler 17.0.1 • Autoloading dependency packages.
	/opt/mpi/intel-18.0.3/mvapich2-2.3/bin/mpirun		module load intel/18.0.3 module load intel-18.0.3/mvapich2/2.3	• Mvapich2 with Intel Compiler 18.0.3 • Autoloading dependency packages.

Application & Library	Binary File & Directory Path	Version	module purge	Remarks
	/opt/mpi/gcc-4.8.5/mvapich2-2.3/bin/mpirun		module load gcc-4.8.5/mvapich2/2.3	• Mvapich2 with GCC 4.8.5
Julia			module load julia/gcc4.8.5/1.0.5 module load julia/gcc-4.8.5/1.8.0 module load julia/gcc-4.8.5/1.6.2 module load julia/gcc-4.8.5/1.9.2	
Python	/opt/python/2.7.15/gcc-4.8.5/bin/python /opt/python/2.7.15/gcc-4.8.5/bin/python2.7	2.7.15	module load tcl+tk/gcc-4.8.5/8.6.9 module load python/gcc-4.8.5/2.7.15	• Python 2.7.5 with GCC 4.8.5 • Autoloading dependency packages.
	/opt/python/3.4.9/gcc-4.8.5/bin/python3 /opt/python/3.4.9/gcc-4.8.5/bin/python3.4	3.4.9	module load tcl+tk/gcc-4.8.5/8.6.9 module load python/gcc-4.8.5/3.4.9	• Python 3.4.9 with GCC 4.8.5 • Autoloading dependency packages.
	/opt/python/3.5.6/gcc-4.8.5/bin/python3 /opt/python/3.5.6/gcc-4.8.5/bin/python3.5	3.5.6	module load tcl+tk/gcc-4.8.5/8.6.9 module load python/gcc-4.8.5/3.5.6	• Python 3.5.6 with GCC 4.8.5 • Autoloading dependency packages.
Python 3.5.6 module list	pygame, PyOpenGL, PyOpenGL-accelerate	3.5.6		
Common python module list	sympy, numpy, scipy, matplotlib, mpi4py, h5py, networkx, qutip, Cython, tables(pytables), pandas, seaborn	-		
kwant	Python module package	1.3.3	module load python/gcc-4.8.5/3.5.6 module load openblas/gcc-4.8.5/0.2.20	• Python 3.5.6 module package. • Manually load dependency packages.
Intel MKL	/opt/intel/2017up1/mkl/lib/intel64/libmkl_intel_lp64.so /opt/intel/2017up1/mkl/lib/intel64/libmkl_sequential.so /opt/intel/2017up1/mkl/lib/intel64/libmkl_core.so /opt/intel/2017up1/mkl/lib/intel64/libmkl_scalapack_lp64.so /opt/intel/2017up1/mkl/lib/intel64/libmkl_blacs_openmpi_lp64.so /opt/intel/2017up1/mkl/lib/intel64/libmkl_blas95_lp64.a /opt/intel/2017up1/mkl/lib/intel64/libmkl_lapack95_lp64.a	17.0.1	module load intel/17.0.1	

	/opt/intel/2018up3/mkl/lib/intel64/libmkl_intel_lp64.so /opt/intel/2018up3/mkl/lib/intel64/libmkl_sequential.so /opt/intel/2018up3/mkl/lib/intel64/libmkl_core.so /opt/intel/2018up3/mkl/lib/intel64/libmkl_scalapack_lp64.so /opt/intel/2018up3/mkl/lib/intel64/libmkl_blacs_openmpi_lp64.so /opt/intel/2018up3/mkl/lib/intel64/libmkl_blas95_lp64.a /opt/intel/2018up3/mkl/lib/intel64/libmkl_lapack95_lp64.a	18.0.3	module load intel/18.0.3	
BLAS	/opt/blas/3.8.0/gcc-4.8.5/lib/libblas.a	3.8.0	module load blas/gcc-4.8.5/3.8.0	• BLAS 3.8.0 with GCC 4.8.5

Application & Library	Binary File & Directory Path	Version	module purge	Remarks
LAPACK	/opt/lapack/3.8.0/gcc-4.8.5/lib/liblapack.a /opt/lapack/3.8.0/gcc-4.8.5/lib/liblapacke.a /opt/lapack/3.8.0/gcc-4.8.5/lib/librefblas.a /opt/lapack/3.8.0/gcc-4.8.5/lib/libtmglb.a	3.8.0	module load lapack/gcc-4.8.5/3.8.0	• LAPACK 3.8.0 with GCC 4.8.5
BLAS+LAPACK	/opt/blas+lapack/3.8.0/gcc-4.8.5/lib/libblas.a /opt/blas+lapack/3.8.0/gcc-4.8.5/lib/liblapack.a /opt/blas+lapack/3.8.0/gcc-4.8.5/lib/liblapacke.a /opt/blas+lapack/3.8.0/gcc-4.8.5/lib/libblas.so /opt/blas+lapack/3.8.0/gcc-4.8.5/lib/libcblas.so /opt/blas+lapack/3.8.0/gcc-4.8.5/lib/liblapacke.so /opt/blas+lapack/3.8.0/gcc-4.8.5/lib/liblapack.so	3.8.0	module load blas+lapack/gcc-4.8.5/3.8.0	• BLAS+LAPACK 3.8.0 with GCC 4.8.5 • Integrated BLAS and LAPACK libraries
CLAPACK	/opt/clapack/3.1.1/gcc-4.8.5/lib/libblas.a /opt/clapack/3.1.1/gcc-4.8.5/lib/liblapack.a /opt/clapack/3.1.1/gcc-4.8.5/lib/libtmg.a	3.1.1.1	module load clapack/gcc-4.8.5/3.1.1.1	• CLAPACK 3.1.1.1 with GCC 4.8.5
	/opt/clapack/3.2.1/gcc-4.8.5/lib/libblas.a /opt/clapack/3.2.1/gcc-4.8.5/lib/liblapack.a /opt/clapack/3.2.1/gcc-4.8.5/lib/libtmglb.a	3.2.1	module load clapack/gcc-4.8.5/3.2.1	• CLAPACK 3.2.1 with GCC 4.8.5
ATLAS	/opt/atlas/3.10.3/gcc-4.8.5/lib/libatlas.a /opt/atlas/3.10.3/gcc-4.8.5/lib/libcblas.a /opt/atlas/3.10.3/gcc-4.8.5/lib/libf77blas.a /opt/atlas/3.10.3/gcc-4.8.5/lib/liblapack.a /opt/atlas/3.10.3/gcc-4.8.5/lib/libptcblas.a /opt/atlas/3.10.3/gcc-4.8.5/lib/libptf77blas.a /opt/atlas/3.10.3/gcc-4.8.5/lib/libatlas.so /opt/atlas/3.10.3/gcc-4.8.5/lib/libcblas.so /opt/atlas/3.10.3/gcc-4.8.5/lib/libsatlas.so /opt/atlas/3.10.3/gcc-4.8.5/lib/libtatlas.so	3.10.3	module load atlas/gcc-4.8.5/3.10.3	• ATLAS 3.10.3 with GCC 4.8.5
BLACS	/opt/blacs/1.1/gcc-4.8.5/openmpi-2.1.5/lib/blacsCinit.a /opt/blacs/1.1/gcc-4.8.5/openmpi-2.1.5/lib/blacsF77init.a /opt/blacs/1.1/gcc-4.8.5/openmpi-2.1.5/lib/libblacs.a	1.1	module load gcc-4.8.5/openmpi/2.1.5 module load blacs/gcc-4.8.5/openmpi-2.1.5/1.1	• BLACS 1.1 with GCC 4.8.5 • For OpenMPI (GCC 4.8.5) • Autoloading dependency packages.

OpenBLAS	/opt/openblas/0.2.20/gcc-4.8.5/lib64/libopenblas.a /opt/openblas/0.2.20/gcc-4.8.5/lib64/libopenblas.so	0.2.20	module load openblas/gcc-4.8.5/0.2.20	• OpenBLAS with GCC 4.8.5
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Application & Library	Binary File & Directory Path	Version	module purge	Remarks
SCALAPACK	/opt/scalapack/2.0.2/gcc-4.8.5/openmpi-2.1.5/lib/libscalapack.so	2.0.2	module load gcc-4.8.5/openmpi/2.1.5 module load blas+lapack/gcc-4.8.5/3.8.0 module load scalapack/gcc-4.8.5/openmpi-2.1.5/2.0.2	• ScaLAPACK 2.0.2 with GCC 4.8.5 • For OpenMPI (GCC 4.8.5) • Autoloading dependency packages.
SuperLU	/opt/superlu/5.2.1/gcc-4.8.5/lib64/libsuperlu.so	5.2.1	module load blas+lapack/gcc-4.8.5/3.8.0 module load superlu/gcc.4.8.5/5.2.1	• SuperLU 5.2.1 with GCC 4.8.5 • Autoloading dependency packages.
Armadillo	/opt/armadillo/9.200.7/gcc-4.8.5/lib64/libarmadillo.so	9.200.7	module load blas+lapack/gcc-4.8.5/3.8.0 module load openblas/gcc-4.8.5/0.2.20 module load atlas/gcc-4.8.5/3.10.3 module load armadillo/gcc-4.8.5/9.200.7	• Armadillo 9.200.7 with GCC 4.8.5 • Autoloading dependency packages.
GSL	/opt/gsl/2.5/gcc-4.8.5/lib/libgslcblas.so /opt/gsl/2.5/gcc-4.8.5/lib/libgsl.so	2.5	module load gsl/gcc-4.8.5/2.5	• GSL 2.5 with GCC 4.8.5
gl2ps	/opt/gl2ps/1.4.0/gcc-4.8.5/lib/libgl2ps.so	1.4.0	module load gl2ps/gcc-4.8.5/1.4.0	• gl2ps 1.4.0 with GCC 4.8.5
arpack	/usr/lib64/libarpack.so	3.1.3	OS default environment.	• RPM Package (with GCC 4.8.5)
byobu	/usr/bin/byobu	5.92-1	OS default environment.	• RPM Package (with GCC 4.8.5)
xmgrace	/usr/bin/xmgrace	5.1.23-4	OS default environment.	• RPM Package (with GCC 4.8.5)
gnuplot	/usr/libexec/gnuplot /usr/bin/gnuplot-wx	4.6.2-3	OS default environment.	• RPM Package (with GCC 4.8.5)
git	/bin/git	2.18.0-1	OS default environment.	• RPM Package
tk-devel	/usr/lib64/libtk.so /usr/lib64/libtkstub8.5.a	8.5.13-6	OS default environment.	• RPM Package
TCL+TK	/opt/tcl+tk/8.6.9/gcc-4.8.5/lib/libtcl8.6.so /opt/tcl+tk/8.6.9/gcc-4.8.5/lib/libtk8.6.so	8.6.9	module load tcl+tk/gcc-4.8.5/8.6.9	• TCL+TK 8.6.9 with GCC 4.8.5

fuse	/usr/bin/fusermount /usr/bin/ulockmgr_server /usr/sbin/mount.fuse	2.9.2	OS default environment.	• OS default Package • User group name fuse • User group GID : 1500 • /dev/fuse owner root:fuse • /dev/fuse permission 666
HDF5	/opt/hdf5/1.8.21/intel-18.0.3/bin	1.10.4	module load intel/18.0.3 module load intel18.0.3/openmpi/2.1.5 module load hdf5/intel- 18.0.3/1.10.4	• For OpenMPI (Intel Compiler 18.0.3) • Autoloading dependency packages.

Application & Library	Binary File & Directory Path	Version	module purge	Remarks
gmp	/opt/gmp/6.1.2/bin	6.1.2	module load gmp/6.1.2	
guile	/opt/guile/2.2.4/gcc-4.8.5/lib/libguile-2.2.so	2.2.4	module load gmp/6.1.2 module load guile/gcc-4.8.5/2.2.4	• guile 2.2.4 with GCC 4.8.5 • Autoloading dependency packages.
libctl	/opt/libctl/4.2.0/intel-18.0.3/lib/libctl.a	4.2.0	module load libctl/intel-18.0.3/4.2.0	• Libctl with Intel Compiler 18.0.3
FFTW	/opt/fftw/3.3.8/intel-17.0.1/single/lib/libfftw3f.so	3.3.8	module load intel/17.0.1 module load fftw/intel-17.0.1/3.3.8/single	• FFTW with Intel Compiler 17.0.1 • Autoloading dependency packages.
	/opt/fftw/3.3.8/intel-17.0.1/double/lib/libfftw3.so		module load intel/17.0.1 module load fftw/intel-17.0.1/3.3.8/double	
	/opt/fftw/3.3.8/intel-18.0.3/single/lib/libfftw3f.so		module load intel/18.0.3 module load fftw/intel-18.0.3/3.3.8/single	• FFTW with Intel Compiler 18.0.3 • Autoloading dependency packages.
	/opt/fftw/3.3.8/intel-18.0.3/double/lib/libfftw3.so		module load intel/18.0.3 module load fftw/intel-18.0.3/3.3.8/double	
Wannier90	/opt/wannier90/2.1.0/intel-17.0.1/intelmpi/bin/postw90.x /opt/wannier90/2.1.0/intel-17.0.1/intelmpi/bin/w90chk2chk.x /opt/wannier90/2.1.0/intel-17.0.1/intelmpi/bin/wannier90.x	2.1.0	module load intel/17.0.1 module load wannier90/intel-17.0.1/intelmpi/2.1.0	• For Intel MPI (Intel Compiler 17.0.1)
	/opt/wannier90/2.1.0/intel-17.0.1/intelmpi/lib/libwannier.a	1.2.0	module load intel/17.0.1 module load wannier90/intel-17.0.1/intelmpi/1.2.0	• For Intel MPI (Intel Compiler 17.0.1)
	/opt/wannier90/1.2.0/intel-17.0.1/intelmpi/bin/wannier90.x /opt/wannier90/1.2.0/intel-17.0.1/intelmpi/lib/libwannier.a			
GLFW	/opt/glfw/3.3/lib64/libglfw.so	3.3	module load glfw/3.3	• GLFW 3.3 with GCC 4.8.5
OpenGL	/opt/OpenGL/3.0/lib/libglfw.so /opt/OpenGL/3.0/lib/libassimp.a /opt/OpenGL/3.0/assimp	3.0	module load OpenGL/3.0	• OpenGL 3.0 with GCC 4.8.5
cmake	/opt/cmake/3.13.2/gcc-4.8.5/bin/cmake /opt/cmake/3.13.2/gcc-4.8.5/bin/ccmake	3.13.2	module load cmake/gcc-4.8.5/3.13.2	• CMake 3.13.2 with GCC 4.8.5
	opt/cmake/3.15.1/gcc-4.8.5/bin/cmake /opt/cmake/3.15.1/gcc-4.8.5/bin/ccmake	3.15.1	module load cmake/gcc-4.8.5/3.15.1	• CMake 3.15.1 with GCC 4.8.5

Application & Library	Binary File & Directory Path	Version	module purge	Remarks
VASP	/opt/vasp/5.4.4/intel-18.0.3/bin/vasp_gam /opt/vasp/5.4.4/intel-18.0.3/bin/vasp_ncl /opt/vasp/5.4.4/intel-18.0.3/bin/vasp_std	5.4.4	module load intel/18.0.3 module load fftw/intel-18.0.3/3.3.8/double module load intel-18.0.3/openmpi/2.1.5 module load vasp/intel-18.0.3/5.4.4	• For OpenMPI (Intel Compiler 18.0.3) • Autoloading dependency packages.
	/opt/vasp/5.4.4/intel-17.0.1/bin/vasp_wannier90_v2.1.0_gam /opt/vasp/5.4.4/intel-17.0.1/bin/vasp_wannier90_v2.1.0_ncl /opt/vasp/5.4.4/intel-17.0.1/bin/vasp_wannier90_v2.1.0_std		module load intel/17.0.1 module load fftw/intel-17.0.1/3.3.8/double module load wannier90/intel-17.0.1/intelmpi/2.1.0 module load vasp/intel-17.0.1/5.4.4	• For Intel MPI (Intel Compiler 17.0.1) • Wannier90 version 2.1.0 • Manually load the wannier90 dependent packages.
	/opt/vasp/5.4.4/intel-17.0.1/bin/vasp_wannier90_v1.2.0_gam /opt/vasp/5.4.4/intel-17.0.1/bin/vasp_wannier90_v1.2.0_ncl /opt/vasp/5.4.4/intel-17.0.1/bin/vasp_wannier90_v1.2.0_std		module load intel/17.0.1 module load fftw/intel-17.0.1/3.3.8/double module load wannier90/intel-17.0.1/intelmpi/1.2.0 module load vasp/intel-17.0.1/5.4.4	• For Intel MPI (Intel Compiler 17.0.1) • Wannier90 version 1.2.0 • Manually load the wannier90 dependent packages.
Quantum Espresso	/opt/espresso/6.3/intel-18.0.3/bin/pw.x	6.3.0	module load intel/18.0.3 module load fftw/intel-18.0.3/3.3.8/double module load intel-18.0.3/openmpi/2.1.5 module load espresso/intel-18.0.3/6.3	• For OpenMPI (Intel Compiler 18.0.3) • Autoloading dependency packages.
meep	/opt/meep/1.7.0/intel-18.0.3/bin/meep	1.7.0	module load intel/18.0.3 module load gmp/6.1.2 module load guile/gcc-4.8.5/2.2.4 module load hdf5/intel-18.0.3/1.10.4 module load fftw/intel-18.0.3/3.3.8/double	• For OpenMPI (Intel Compiler 18.0.3) • Autoloading dependency packages.

			module load libctl/intel-18.0.3/4.2.0 module load intel-18.0.3/openmpi/2.1.5 module load meep/intel-18.0.3/1.7.0	
texlive	/opt/texlive/2018/bin/x86_64-linux/tex	2018	module load texlive/2018	
MATLAB	/opt/MATLAB/R2017b/bin/matlab /opt/MATLAB/R2020b/bin/matlab /opt/MATLAB/R2022a/bin/matlab	R2017b R2020b R2022a	module load matlab/R2017b module load matlab/R2020b module load matlab/R2022a	
Mathematica	/opt/Wolfram/Mathematica/11.0/Executables/mathematica /opt/Wolfram/Mathematica/12.1 /Executables/mathematica	11.0 12.1	module load mathematica/11.0 module load mathematica/12.1	
Blender	/opt/blender/2.79b/blender	2.79b	module load blender/2.79b	
Intel oneAPI Base & HPC Toolkit	/opt/Modules/compiler/intel-oneapi	2021.2	module purge module load intel/mkl-2019u5 module load advisor/2022.0.0 module load debugger/latest module load icc32/2022.0.2 module load mkl/latest module load advisor/latest module load dev-utilities/2021.5.2 module load icc32/latest module load mkl32/2022.0.2 module load ccl/2021.5.1 module load dev-utilities/latest module load init_oneapi/2022.0.2 module load mkl32/latest module load ccl/latest module load dnnl/2022.0.2 module load init_oneapi/latest module load mpi/2021.5.1	Support Period End: 2023-01-05

		module load clck/2021.5.0 module load dnnl/latest module load inspector/2022.0.0 module load mpi/latest module load clck/latest module load dnnl-cpu-gomp/2022.0.2 module load dnnl-cpu-gomp/latest module load dnnl-cpu-iomp/2022.0.2 module load dnnl-cpu-iomp/latest module load inspector/latest module load oclfpga/2022.0.2 module load compiler/2022.0.2 module load dnnl-cpu-gomp/latest module load intel_ipp_ia32/2021.5.2 module load oclfpga/latest module load compiler/latest module load dnnl-cpu-iomp/2022.0.2 module load intel_ipp_ia32/latest module load tbb/2021.5.1 module load compiler-rt/2022.0.2 module load dnnl-cpu-iomp/latest module load intel_ipp_intel64/2021.5.2 module load tbb/latest module load compiler-rt/latest module load dnnl-cpu-tbb/2022.0.2 module load intel_ipp_intel64/latest module load tbb32/2021.5.1 module load compiler-rt32/2022.0.2 module load dnnl-cpu-tbb/latest module load intel_ippcp_ia32/2021.5.1 module load tbb32/latest module load compiler-rt32/latest module load dpct/2022.0.0	
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			module load intel_ippcp_ia32/latest module load vpl/2022.0.0 module load compiler32/2022.0.2 module load dpct/latest module load intel_ippcp_intel64/2021.5.1 module load vpl/latest module load compiler32/latest module load dpl/2021.6.0 module load intel_ippcp_intel64/latest module load vtune/2022.0.0 module load dal/2021.5.3 module load dpl/latest module load itac/2021.5.0 module load vtune/latest module load dal/latest module load icc/2022.0.2 module load itac/latest module load debugger/2021.5.0 module load icc/latest module load mkl/2022.0.2 module load llvm/8.0.0 source /opt/intel/oneapi/setvars.sh	
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