

Plumed

Dostupne verzije su:

Verzija	Modul
2.5.2	plumed/2.5.2
2.7.2	plumed/2.7.2
2.7.3	plumed/2.7.3
2.8.0	plumed/2.8.0

Instalacija

Instalacija je prevedena s Intel 2019 i MVAPICH 2.2 i parametrima:

```
module load mpi/mvapich2-intel-2.2-x86_64
export CC=mpicc
export CXX=mpicxx
export F77=mpif77
export F90=mpif90
export FC=mpif90
export CFLAGS="-O3 -I/opt/intel/mkl/include/intel64/ilp64 -I/opt/intel/mkl/include -I/opt/intel/mkl/include
/fftw -mkl"
export LIBS="-O3 /opt/intel/mkl/lib/intel64/libmkl_blas95_ilp64.a /opt/intel/mkl/lib/intel64
/libmkl_lapack95_ilp64.a -L/opt/intel/mkl/lib/intel64 -lmkl_scalapack_ilp64 -lmkl_intel_ilp64 -lmkl_sequential -
lmkl_core -lmkl_blacs_intelmpi_ilp64 -lpthread -lm -ldl"
# install
./configure --prefix=/apps/plumed/2.5.2
make
make install
```