

Abinit

Abinit je preveden s Intel 2019 i MVAPICH2 2.2 i parametrima:

```
./configure CC=mpicc CXX=mpicxx FC=mpif90 FCFLAGS="-O2" CFLAGS="-O2" CXXFLAGS="-O2" --with-fc-vendor=intel -  
with-fft-flavor=fftw3-mkl --with-fft-libs="-lmkl_intel_lp64 -lmkl_sequential -lmkl_core" --with-linalg-  
flavor=mkl --enable-mpi --with-mpi-prefix=/usr/lib64/mvapich2-intel-2.2 --enable-64bit-flags --disable-debug --  
with-dft-flavor="none" --with-trio-flavor="none" --enable-mpi-inplace --enable-mpi-io --prefix=/apps/abinit  
/VERSION  
make  
make install
```

Dostupne verzije su:

Verzija	Modul
8.8.4	abinit/8.8.4
8.10.2	abinit/8.10.2

Primjer korištenja:

```
module load abinit/8.8.4  
mpirun -np $NSLOTS -genv MV2_ENABLE_AFFINITY 0 -machinefile $TMPDIR/machines abinit -i input_files
```