

Dalton

Dalton 2018 je preveden s Intel 2019 i MVAPICH2 2.2 i parametrima:

```
./setup --fc=mpif90 --cc=mpicc --cxx=mpicxx --cmake=cmake3 --mpi --scalapack
```

Dalton 2020 je preveden s GCC 4.8.5 i openmpi31 i parametrima:

```
./setup --fc=mpif90 --cc=mpicc --cxx=mpicxx --cmake=cmake3 --mpi
```

Dostupne verzije su:

Verzija	Modul
2018	dalton/dalton_2018
2020	dalton/dalton_2020
2020	dalton/dalton_2020_custom

Primjer korištenja:

```
module load dalton/dalton_2018

export DALTON_TMPDIR=$TMPDIR
export DALTON_LAUNCHER="mpirun -np $NSLOTS -hostfile $TMPDIR/machines"

dalton -d -mb 16000 -ow -noarch TEST TEST
```



Aplikacija Dalton maksimalno može koristiti 16GB radne memorije, više na linku <http://forum.daltonprogram.org/viewtopic.php?f=9&t=816>

Custom verzija je prevedena s drugačijim parametrima u include datotekama

```
/DALTON/include/rspprp.h
MAXLBL = 30000

/DALTON/include/infvar.h
MAXWOP = 1500000

/DALTON/include/maxorb.h
MXSHEL = 8000
MXCORB = 7000

/DALTON/include/aovec.h
MXAOVC = 72
```