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#!/bin/tcsh
#SBATCH -N 1
#SBATCH -n 4
#SBATCH --mem 5000
#SBATCH -p standard
module load ifort
module load mkl
#module load openmpi/4.1.0_gcc620
#module load fftw/3.3.8_gcc620
setenv LD_LIBRARY_PATH
{ $LD_LIBRARY_PATH }:/home/users/mollabashi/expand/fftw/lib:/home/users/mollabashi/expand/openmpi/lib
setenv PATH { $PATH }:/home/users/mollabashi/expand/openmpi/bin/
setenv WIENROOT /home/users/mollabashi/expand/v21.1
which mpirun
which lapw1
echo $PATH
echo $WIENROOT
echo $LD_LIBRARY_PATH
ldd $WIENROOT/lapw1_mpi
ldd $WIENROOT/lapw0_mpi
rm -fr .machines
# for 24 cpus and kpoints (in input file)
# #write .machines file
# #echo '#' .machines
# # example for an MPI parallel lapw0
echo 'lapw0:`hostname`:2' >> .machines
echo '1:`hostname`:2' >> .machines
echo '1:`hostname`:2' >> .machines
echo 'granularity:1' >>.machines
echo 'extrafine:1' >>.machines
x lapw0
x lapw0 -p

```