```
#!/bin/bash
# # In this script one comment before SBATCH is for enable option
# # two comment before SBATCH is for disable option

#****** OPTIONS TO CHANGE IN PRIORITY ******
# -p : queue    - defq (default): unlimited
#       - express (15 min & 4 nodes max)
# -n : processors (20 per node in defq and express)
# -N : nodes
# -t : walltime (format h:mm:ss): default is 12h
# --mem=<memory in Megabytes> : 64 GB per node (3.2 GB per core) on defq
# --mem-per-cpu=2048M  :3.2 GB per CPU on defq
# --exclusive : Job allocation can not share nodes with other running jobs

#SBATCH -J titre de mon calcul
#SBATCH -p kernel3
#SBATCH -n 20
#SBATCH -N 1
#SBATCH -t 120:00:00
##SBATCH --mem=256000
##SBATCH --mem-per-cpu=2048M
##SBATCH --exclusive


SEEDNAME=moncompose_optimise
SEEDNAME2=$SEEDNAME\_NMR

curentdir="$PWD"


#****** OTHER (LESS-IMPORTANT OPTIONS TO CHANGE OPTIONALLY ********
# -J : job name
# --mail-type=ALL : Send mail: valid types are BEGIN, END, FAIL, REQUEUE, and ALL
# --mail-user=user@cnrs-orleans.fr
# --output slurm-%j.txt : Write stdout output, %j is replaced with the job number
# --error slurm-%j.txt : Write stderr output, %j is replaced with the job number
#           use same path name to write everything to one file
# --workdir=<directory> : Set the working directory of the batch script to directory before
it is executed
# --exclusive

echo Running on $(hostname)
echo Available nodes: $SLURM_NODELIST
echo Slurm_submit_dir: $SLURM_SUBMIT_DIR
echo Start time: $(date)
echo Job ID: $SLURM_JOB_ID
#
# If you want to use the SCRATCH Filesystem
# you may add commands to your batch script to copy data
#in $SCRATCH at the beginning of a run and copy out at the end.
# The SCRATCH Filesystem is better for I/O Job
#
SCRATCH=/scratch/$USER/$SLURM_JOB_ID
#create your SCRATCH directory
mkdir $SCRATCH
# Copy all input files to your scratch directory
cp $SLURM_SUBMIT_DIR/* $SCRATCH/.
```

```
cd $SCRATCH
echo "Files accessible during runtime (read-only) in dir.: $SCRATCH"

#load environment modules
module purge
module load shared
module load slurm gcc openmpi/intel/64/1.8
module load MaterialStudio/8.0

# Write here your command line
#mpirun <executable> <arguments>
#or
#mpirun $SCRATCH/<executable> <arguments>
mpirun castep.mpi $SEEDNAME
  echo "CASTEP MPI job : start NMR Calculation"
  cp $SLURM_SUBMIT_DIR/$SEEDNAME2.cell .
  cp $SLURM_SUBMIT_DIR/$SEEDNAME2.param .
  mv $SEEDNAME.check $SEEDNAME2.check
  mpirun castep.mpi $SEEDNAME2


#If you used the SCRATCH Filesystem
# Copy all OUTPUT files to your home directory
mkdir $SLURM_SUBMIT_DIR/result_$SLURM_JOB_ID
cp $SCRATCH/* $SLURM_SUBMIT_DIR/result_$SLURM_JOB_ID/.

#Remove your scratch folder
rm -fr $SCRATCH
```