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#!/bin/bash

### This is a SBATCH submission file.
### MON_JOB will run on 8 processors for a maximun of 48 hours on the
defq queue.
### The pimaim (parallel code for classical MD calculations) job need
ifort and openmpi environment.
### The job use home directory.

### Nom du job
#SBATCH -J 3pc_UF4-ThF4-LiF_975K

### Nombre de processeurs
#SBATCH -n 8

### Nombre de noeuds
#SBATCH -N 1

###The job allocation can not share nodes with other running jobs
###SBATCH --exclusive

### memoire requise par noeud (megabytes)
###SBATCH --mem=256000

### Duree maxi du job
#SBATCH -t 48:00:00

### file d attente (defq ou express)
#SBATCH -p defq

###module load shared
module load intel/compiler/64/15.0/2015.0.090 intel/openmpi-for-intel/1.8

echo Running on $(hostname)
echo Available nodes: $SLURM_NODELIST
echo Slurm_submit_dir: $SLURM_SUBMIT_DIR
echo Start time: $(date)

### Write stdout/stderr output, %j is replaced with the job number
###SBATCH --output slurm-%j.txt
###SBATCH --error slurm-%j.txt

mpirun ./pimaim_mpi_thermal.exe
```