Compiling and Using MPI CP2K on UB-CCR

05/30/20

1. git clone --recursive https://github.com/cp2k/cp2k.git cp2k
2. cd tools/toolchain/
3. source /util/academic/intel/19.5/compilers_and_libraries_2019.5.281/linux/mkl/bin/mklvars.sh intel64
4. module load openmpi/3.0.3/gcc-7.3.0
5. conda deactivate
6. ./install_cp2k_toolchain.sh --with-libint=no --with-libxc=no --with-elpa=no --with-sirius=no --with-hdf5=no --with-libxsmm=no
7. cp /path/to/cp2k/tools/toolchain/install/arch/* ../../arch
8. source /path/to/cp2k/tools/toolchain/install/setup
9. cd ../../
10. make -j 32 ARCH=local VERSION="popt"

Step 5 many not be required for all. But sometimes when building the FFTW library the build uses Conda paths for some reason and the compilation crashes. When deactivating Conda it works.

the code can be run from the terminal as:
mpirun -n 4 /path/to/cp2k.popt -i cp2k_input_file_here

Strange Occurrences:

For some reason when I submit to the faculty nodes it crashes. But when I submit to the ub-hpc nodes it runs fine. I read online that this could be due to the different types of processes of the nodes. Basically, this cp2k package (the one herein) is built for a particular processor type, making it incompatible with processors on the faculty cluster. Below is the error I get when submitting to the faculty cluster. The code runs fine on ub-hpc.

```
SLURM_JOBID=2063248
SLURM_JOB_NODELIST=cpn-f11-06
SLURM_NNODES=1
SLURMTMPDIR=/scratch/2063248
working directory=/gpfs/scratch/brendan/cp2k_test/test_sp_tddft

Program received signal SIGILL: Illegal instruction.

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Backtrace for this error:

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Backtrace for this error:
#0  0x2b49d708a3af in ???
#0  0x2b5d19d293af in ???
#1  0x4f8809 in cp2k
        at /gpfs/scratch/brendan/cp2k/src/start/cp2k.F:96
#2  0x4f86dc in main
        at /gpfs/scratch/brendan/cp2k/src/start/cp2k.F:45
#1  0x4f8809 in cp2k
        at /gpfs/scratch/brendan/cp2k/src/start/cp2k.F:96
#2  0x4f86dc in main
        at /gpfs/scratch/brendan/cp2k/src/start/cp2k.F:45
--------------------------------------------------------------------------
Primary job  terminated normally, but 1 process returned
a non-zero exit code. Per user-direction, the job has been aborted.
--------------------------------------------------------------------------
#0  0x2b0392f343af in ???
#1  0x4f8809 in cp2k
        at /gpfs/scratch/brendan/cp2k/src/start/cp2k.F:96
#2  0x4f86dc in main
        at /gpfs/scratch/brendan/cp2k/src/start/cp2k.F:45
--------------------------------------------------------------------------
mpirun noticed that process rank 1 with PID 29674 on node cpn-f11-06 exited on signal 4 (Illegal instruction).
--------------------------------------------------------------------------
```

SOLUTION BELOW

Using #SBATCH --constraint=CPU-Gold-6130 works. It appears that this was the processor I used to compile cp2k. Therefore, make sure set the correct processor constraint in your slurm submit file. The next page is my slurm file for reference. Unfortunately, this constraint prohibits the use of the Valhalla partition.

```
#!/bin/sh
###SBATCH --partition=valhalla  --qos=valhalla
###SBATCH --clusters=faculty
#SBATCH --partition=scavenger  --qos=scavenger
#SBATCH --clusters=faculty
#SBATCH --constraint=CPU-Gold-6130
#SBATCH --time=72:00:00
#SBATCH --nodes=1
#SBATCH --requeue
#SBATCH --ntasks-per-node=12
#SBATCH --cpus-per-task=1
#SBATCH --mem=75000
#SBATCH --mail-user=bsmith24@buffalo.edu

echo "SLURM_JOBID="$SLURM_JOBID
echo "SLURM_JOB_NODELIST="$SLURM_JOB_NODELIST
echo "SLURM_NNODES="$SLURM_NNODES
echo "SLURMTMPDIR="$SLURMTMPDIR
echo "working directory="$SLURM_SUBMIT_DIR

module load openmpi/3.0.3/gcc-7.3.0
export I_MPI_PMI_LIBRARY=/usr/lib64/libpmi.so

srun /gpfs/scratch/brendan/cp2k/exe/local/cp2k.popt -i Th.inp -o Th.out
```