HPC usage guide for Gaussian 16 on jakar.utep.edu

Gaussian 16 version B.01 with AVX2 support and Linda executables are installed under /shared/gaussian/g16

In order submit a g16 calculation to the cluster one needs to prepare a submit script in the same directory as the input file(s) for the calculation.

Gaussian 16 does not recognize the runtime environment when the calculation starts. This especially important for smaller calculations when only a small number of CPU cores are needed for parallel execution.

It is required to set the %NProcShared value to the number of cores in the input file's Link 0 section, as well as the %MEM value. Here is an example:

```
%chk=mol-opt-nbo.chk
%Mem=16GB
%NProcShared=2
```

The values in the submit script need to correspond to the %NProcShared value.
Here is an example for a corresponding submit script:

```
#!/bin/bash
#SBATCH -n 2
#SBATCH --threads-per-core=1
#SBATCH --partition=chem
# Gaussian 16 root directory
export g16root="/shared/gaussian/"
#
# Load the gaussian profile file
. ${g16root}/g16/bsd/g16.profile
#
# Scratch directory
export GAUSS_SCRDIR="$HOME/scratch"
#
# Run G16 job
g16 < mol-opt-nbo.gjf >& mol-opt-nbo.log
```

The -n 2 on top is the number of requested cores.

The next line will prevent linux to use Intel's hyperthreading which actually will slow down gaussian, according to their documentation.

The partition setting sets the segment of the cluster.

All commands before the actual g16 command will set the Gaussian environment, for executables and other environment variables.

Scratch is set to /home/<username>/scratch

Make sure the scratch directory exists and is fully accessible for writing and reading data.

The last list is the actual g16 command.

Submit the job with the command:

```
sbatch < submit.sh
```

Check the status of the job with the command:

```
squeue
```

All output files will be written to the directory from which you submitted the job.