


Gaussian

Purpose: Electronic Structure Calculations
Latest version: Gaussian16 C.02
License:  Provided by CSUC
Closed-source
Website: http://gaussian.com/_ext-link

Gaussian is a program implementing a variety of computational chemistry methods.

The range of computational methods includes molecular mechanics, semi-empirical methods, Hartree-Fock SCF, Møller-Plesset perturbation theory, DFT methods, QM/MM calculations, CI methods and CC calculations. Calculations employing these methods can be carried out in order to optimise molecular geometry, electronic structure and derived chemical properties.

SLURM Submit script example

More information about the submit script can be found using the *Job Script Generator*.

Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the *sbatch command page*.

- **-J:** Name for the job's allocation.
- **-e:** Name of the stderr redirection filename.
- **-o:** Name of the stdout redirection filename.
- **-p:** Name of the partition (queue) where the job will be submitted.

gaussian_example.slm

```
#!/bin/bash
#SBATCH -J gaussian_example
#SBATCH -e gaussian_example.%j.err
#SBATCH -o gaussian_example.%j.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -c 4
#SBATCH -t 0-02:00

module load apps/gaussian/g16b01

##
# Modify the input and output files!
INPUT_FILE=gaussian_example.com
OUTPUT_FILE=gaussian_example.log

##
# You don't need to modify nothing more
cp -r ${SLURM_SUBMIT_DIR}/${INPUT_FILE}
${SCRATCH}
cd ${SCRATCH}

srun g16 < ${INPUT_FILE} > ${OUTPUT_FILE}

cp ./${OUTPUT_FILE} ${SLURM_SUBMIT_DIR}
```

- **-n**: Number of tasks.
- **-c**: Number of cores per task.
- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.

Software execution information:



We do not support Linda, so MPI parallelization is not available. This implies that:

- The number of tasks must be 1 (**-n** flag).
- **-c** flag must have the same value as **%nprocs** in the Gaussian input file.
- **--mem** must be higher than the value defined as **%mem** in *input.com* file. More info *here*.

Tutorial

You can follow *this tutorial* about geometric optimisation with Gaussian to get hands-on with the program.
