GAMESS

Purpose: Electronic Structure Calculations
Latest version: 2018
Licence: Free of use
Free of charge research licence _ext-link
Website: *http://www.msg.ameslab.gov/_ext-link*

GAMESS is a program for ab initio molecular electronic structure calculations.

Functionality includes HF, GVB, MCSCF, CI, MP2, CC and DFT methods, excited states, geometry optimisation, vibrational frequencies, solvation effects, relativistic corrections, pseudopotentials and nuclear wavefunctions.

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 sterr redirection filename.
- **-o**: Name of the stdout redirection filename.
- **-p**: Name of the partition (queue) where the job will be submited.
- **-n**: Number of tasks.
- **-c**: Number of cores per task.

gamess_example.slm

```
#!/bin/bash
#SBATCH -J gamess_example
#SBATCH -e gamess_example.err
#SBATCH -o gamess_example.out
#SBATCH -p std
#SBATCH -n 1
#SBATCH -t 0-02:00

module load apps/gamess/2018
source /prod/comp/intel/2018.1.163/linux/bin
/compilervars.sh intel64

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

cp -r ${SLURM_SUBMIT_DIR}/${INPUT_FILE}
${SCRATCH}
cd ${SCRATCH}

srun rungms.slurm ${INPUT_FILE}

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

- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.