ORCA

Purpose: electronic Structure Calculations
Latest version: 5.0.4
License: ✅ Free of use for academics
Mixed
Website: *https://orcaforum.kofo.mpg.de/_ext-link*

ORCA is a program that implements HF, DFT, semi-empirical, and high level ab initio (CI and CC) methods with gaussian basis sets for electronic structure calculations.

ORCA implements a variety of standard quantum chemistry methods, but is especially tailored at geometry optimisation and prediction of spectroscopic parameters in open-shell molecular systems. It can be coupled to ***Gromacs*** for QM/MM calculations.

SLURM Submit script example

For more information use 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.

orca_example.slm

```
#!/bin/bash
#SBATCH -J orca_example
#SBATCH -e orca_example.err
#SBATCH -o orca_example.out
#SBATCH -p std
#SBATCH --ntasks=4
#SBATCH -t 02-00:00

module load apps/orca/4.1.0

##
#  Modify the input and output files!
INPUT_FILE=orca_example.inp
OUTPUT_FILE=orca_example.out

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

$(which orca) ${INPUT_FILE} > ${OUTPUT_FILE}

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

    - For parallel calculations, the number of processes must be explicitly indicated in orca_example.inp file using:

      ```
      %pal nprocs 4 end
      ```

- **-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:

ORCA uses 3000MB per core by default. This value can be changed in orca_example.inp using the directive:

```
%maxcore 3000 end
```

It is recommended to use ~75% of the requested memory to SLURM, which is 3990 MB per core.