

ADF

Purpose: Density Functional Theory

Latest version: 2021.104

License: ⚠️ Must be provided by the user.

Proprietary License _ext

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Website: <https://www.scm.com/>

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Amsterdam Density Functional (ADF) is a proprietary software suite for density functional theory (DFT) calculation of molecular systems, especially inorganic systems.

ADF implements Kohn-Sham-type DFT calculations to finite molecular systems, in gas phase or in solution. It applies LDA, GGA, and in some cases hybrid and meta-GGA functionals, including relativistic effects, to Slater-type orbitals.

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.
- **-n:** Number of tasks.

adf_example.slm

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

module load apps/adf/2019.103

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

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

adf ${INPUT_FILE} ${OUTPUT_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.