

## NWChem

**Purpose:** Electronic Structure Calculations

**Latest version:** 6.8

**License:**  Free of use  
*EDL \_ext-link*

**Website:** *http://www.nwchem-sw.org/\_ext-link*

NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters.

## SLURM Submit script example

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

### nwchem\_example.slm

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

module load apps/nwchem/6.8

##
# Modify the input and output files!
INPUT_FILE=nwchem_example.in
OUTPUT_FILE=nwchem_example.out

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

srun nwchem ${INPUT_FILE} > ${OUTPUT_FILE}

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

## 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.
- **-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.
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