Q-Chem on HPC

What is Q-Chem?

Q-Chem 5.3.2 is a quantum chemistry software program used to perform simulations and calculations of chemical systems. It is a powerful tool for calculating various properties of molecules, including their electronic structure, spectroscopy, and reactivity. The software is equipped with a range of advanced quantum mechanical and quantum chemical methods, including density functional theory, post-Hartree-Fock methods, and semi-empirical approaches. Q-Chem is widely used in the computational chemistry community, and it is often used in conjunction with experimental studies to gain insight into chemical reactions and processes.

Links:

Official Website

Documentation

Manual

Versions Available:

The following versions are available on the cluster:

- qchem_5.3.2 MPICH3

How to load Q-Chem?

To load Q-Chem, use the following commands:

```
#Load the Q-Chem module
module load qchem_5_3
```

To verify if the module is loaded correctly, use the following command,

```
# List all the module loaded in the environment
module list
```

In a fresh environment, this should show Intel Compiler and Q-Chem as loaded modules.

How to use Q-Chem?

In this step, you need to prepare input files that specify the details of the quantum chemical calculation you want to perform. The input file format for Q-Chem is a plain text file that follows a specific syntax. Some of the key parameters that need to be specified in the input file are:

1. Chemical system: The chemical system to be studied, including the molecular structure and any relevant chemical reactions.
2. Quantum mechanical method: The quantum mechanical method to be used for the calculation, such as density functional theory (DFT) or Hartree-Fock (HF).
3. Basis set: The basis set to be used for the calculation, such as Gaussian or Slater-type orbitals.
4. Calculation type: The type of calculation to be performed, such as a geometry optimization or a frequency calculation.
5. Computational resources: The computational resources required for the calculation, such as the number of processors, memory, and wall-clock time.

It is important to thoroughly understand the input file format and the various parameters that can be specified in order to prepare accurate and efficient input files for your calculations. See **specific software documentation** for more information.

Here is a sample input files for testing,

```
$molecule
0 1
```

```
C
H 1 r
H 2 r r_angle
$end

$rem
JOBTYPE freq
EXCHANGE b3lyp
BASIS 6-31g*
SCF_CONVERGENCE 8
SYMMETRY false
$end

$frequency
$end
```

Since this software can be parallelized or run on GPU, use the following template slurm script to submit the job,

```
#!/bin/bash
#THIS IS A THREADED SCRIPT
#SBATCH --p main
#SBATCH --qos main
#SBATCH --job-name=qchem_freq
#SBATCH --ntasks=12
#SBATCH --mem=32GB
#SBATCH --time=12:00:00
#SBATCH --output=qchem_freq.out

module load qchem_5_3
qchem -nt $NTASKS qchem_input.in qchem_output.out
```

Here is another MPI job script,

```
#!/bin/bash
#SBATCH -N 2
#SBACTH -n 32
#SBATCH -t 00:30:00
#SBATCH -J my_job
#SBATCH  -p main
#SBATCH --qos main

module load qchem_5_3
qchem -slurm -mpi -np 2 -nt 32 B3LYP_water.in
```

Users are recommended to read the software documentation on official website,

Where to find help?

If you are confused or need help at any point, please contact OIT at the following address.

https://ua-app01.ua.edu/researchComputingPortal/public/oitHelp