Orca on HPC

What is Orca?

ORCA is a quantum chemistry software package that uses advanced electronic structure methods to calculate the properties of molecules and materials. It includes density functional theory, many-body perturbation theory, coupled cluster theory, multireference methods, and semi-empirical quantum chemistry methods. These methods allow for the prediction of various chemical and physical properties of a system such as energy, geometry, spectra and properties. ORCA is widely used in the computational chemistry community and has a large user base.

Links:

Official Website

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Versions Available:

The following versions are available on the cluster:

- physical/orca/4.2.0
- physical/orca/5.0.1
- physical/orca/5.0.2
- physical/orca/5.0.3

How to load Orca?

To load Orca, use the following commands:

```
#Load the Orca module
module load physical/orca/5.0.3
```

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 gcc, openmpi and orca loaded.

How to use Orca?

To use orca in HPC, users need to first acquire permission to use the software. After getting the permissions, they get access to executable files.

Here is a general demonstration of usage of orca. Follow the steps in the website and prepare the input file,

ORCA demo

To submit the job to the slurm, use the following script as reference

```
#!/bin/bash
#SBATCH --job-name=ORCA_DEMO
#SBATCH --output=thi_05.slurmout
#SBATCH --partition= main
#SBACTH --qos main
#SBATCH --nodes=1
#SBATCH --ntasks=8
#SBATCH --ntasks-per-socket=4
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2000

# Load the module
 module load physical/orca/5.0.3

orca input.inp > output.out
```

```
This is just a sample. Feel free to modify the script as per needed.
```

To see more information about the software, use the official website as reference.

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