

Gaussian on HPC clusters:

About Gaussian:

Gaussian is a computational chemistry software toolkit initially released in 1970. It is used in a wide range of fields including engineering, biology, chemistry, physics, and others. The newest version of gaussian packs advances in modeling and computational capabilities, which makes it a top choice to investigate real-world chemical problems.

The fundamental domain gaussian works are handling quantum mechanical problems like predicting vibrational frequencies, molecular structure, and properties of compounds, predicting the energy state, and so on. Moreover, gaussian can be used to model and predict the compounds and elements which are practically impossible to work within a lab due to their chemical properties.

<https://gaussian.com/>

Versions available on UAHPC:

Gaussian v16.a03

Gaussian v09.d01

Gaussian v03.e01

How to load Gaussian?

If needed, one can unload an existing module loaded on your terminal session, use the following command:

```
module unload <module name>
```

To load the gaussian on your session, enter the following command on your terminal session.

- `module load gaussian/g16.a03`
- `module load gaussian/g09.d01`
- `module load gaussian/g03.e01`

How to build a Molecule?

If your terminal has X11 forwarding, GUI applications can be rendered from the cluster to your screen.

agui {output file}

This command will open a GUI for building input files or viewing output files.

NOTE: Please use the compute nodes to run a GUI session if you can. Try not to use the head node for this task.

One can launch an interactive session for running AGUI on a compute node by running:

```
srun -p main --qos main --ntasks-per-node=1 --mem-per-cpu=4G -pty bash
```

```
module load gaussian/g16.a03
```

```
agui
```

Example input file

The contents of example.com used as a reference file is listed below.

```
%chk=example
```

```
# HF/6-31G(d)
```

```
water energy
```

```
0 1
```

```
O -0.464 0.177 0.0
```

```
H -0.464 1.137 0.0
```

```
H 0.441 -0.143 0.0
```

Note: The file extension we use for processing is .com instead of .gjf

Interactive script:

After loading the gaussian module, example Gaussian job submission scripts will be sourced in your PATH. The following is the syntax for processing a gaussian script. Simply type this on your terminal session:

```
rung16 example.com
```

Note: Do not use extra flags or directives

A prompt will ask how many cores you would like to use for the calculation. There are other flavors of the interactive script that are pre-built. For example, if one wishes to run Gaussian on the long queue, `rung16.long` script is readily available.

Tweaking the script:

If you want to customize the script for your specific needs, the files are in the following directory:

```
/share/apps/gaussian/scripts
```

Simply, copy them into your home directory and use a text editor to tweak the parameters.

After the job is completed, the following files are written to your directory.

```
example.chk example.err example.log
```

To view a log file, use a text editor of choice. For example:

```
nano example.log
```

Alternatively, one can use the AGUI GUI to view the resulting `.log` file.

Where to find help?

If you are stuck on some part or need help at any point please contact at the following address.

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