Gaussian & GaussView

- Gaussian and GaussView are available on the cluster via the environment module system.
- Due to licensing regulations, access is limited to authorized users who have explicitly accepted the terms of use.
- The older (non-default) software version (g16.A03) is incompatible with AMD cpus.

Requesting Access (License Agreement)

Gaussian requires all users to formally confirm and adhere to the following licensing rules:

- **Academic References**: Publications of results achieved using a specific version and revision of Gaussian must always include appropriate references (found in the log files or online).
- **Non-Weapon Clause**: The software must not be used for the development or production of biological or chemical weapons.

To request access, please send an email to **cluster-help@luis.uni-hannover.de** with your **cluster account name** using the template below:

Subject: Request to be added to the group of Gaussian users

Body: Please add my user account **<your_account_name>** to the group of Gaussian users.

I agree to be bound by Gaussian's licence agreement that requires publications of results achieved using a specific version and revision of Gaussian to always include appropriate references, which I can find in the log files of Gaussian jobs or online. Furthermore, I confirm that I will not use the software for the development or production of biological or chemical weapons.

We apologize for the inconvenience, but these are the licensing terms we are legally required to enforce.

After you are added to the Gaussian group (you can check your groups using the `id` command), you should be able to load the modules and proceed.

Loading the Module

Gaussian and GaussView are provided as separate modules. To load the software in your environment, use the standard module commands:

```
# To load Gaussian
```

```
module load Gaussian

# To load GaussView
module load GaussView
```

The latest supported version installed on the cluster is **Gaussian 16 version B01**.

Access Error

If your account is not a member of the authorized user group, the loading process will fail with an error message like the following:

```
Lmod has detected the following error:
You do not have access to this module. Contact cluster-help@luis.uni-
hannover.de
While processing the following module(s):
    Module fullname   Module Filename
    ---------------   ---------------
    Gaussian/g16.B01  /sw/apps/modules/noarch/all/Gaussian/g16.B01.lua
```

If you encounter this error, please request to be added to the group of Gaussian users following the steps above.

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https://docs.cluster.uni-hannover.de/doku.php/guide/soft/gaussian

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