Max-Planck-Institut für Polymerforschung
Max Planck Institute for Polymer Research

Chemical Software

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Gaussian / GaussView

Please note: to use Gaussian, your account has to be a member of the "gaussian" group. Please mail helpdesk (helpdesk@mpip-mainz.mpg.de) to add you to it.

Gaussian 16

Gaussian 16 binaries have been installed in `/sw/linux/gaussian/g16`. To be able to use it on the thinc cluster please set the following environment variables in your Job script:

```
export g16root=/sw/linux/gaussian/g16
. $g16root/g16/bsd/g16.profile

export GAUSS_SCRDIR=/usr/scratch/$LOGNAME
```

For interactive use, set *`g16root`* in your `.profile` or `.bashrc` and run the rest in the terminal you're running Gaussian in (or script you're using). Please remember to log off and on again, after changing `.profile` and/or `.bashrc`.

The g16 initialization script sets up an alias "gv" which points to GaussView.

Example SLURM job script

This is an example of a job script for gaussian. Partially half-inched from the documentation for the "stallo" cluster of UiT The Arctic University of Norway.

```
#!/bin/bash -l

#                   (_)
#  SLURM Options    <) )>
```

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```
################### / \

# Define the partition on whoch the job will run.  Defaults to
# CPU_Std32 if omitted.
# Partitions currently (December 2023) are:
# - CPU_Std20
# - CPU_Std32
# - CPU_IBm32
# - GPU_Std16
#SBATCH --partition=CPU_Std20


# Define, how many nodes you need. Here, we ask for 1 node.
# Only the COU_IBm32 partition ca use mor then one node
#SBATCH --nodes=1


# Number of cores (i.e. 'rank' in MPI) (defaults to 1, if omitted):
#SBATCH --ntasks=20


# mails? and to whom
#SBATCH --mail-type=END,FAIL
# SBATCH --mail-user=YOUR_ACCOUNT_NAME@mpip-mainz.mpg.de

################################################################################
# no bash commands above this line
# all sbatch directives need to be placed before the first bash command


# name of the input file without the .com extention
input=example


## get path to submission directory:
submission_directory=$(scontrol show job "$SLURM_JOB_ID" \
                           | grep -E '^[[:blank:]]*Command=' \
                           | cut -d= -f2 | xargs dirname)


## don't change this:
scratch_directory_base="/usr/scratch/${LOGNAME}"

## use the job id for temporary directory
working_directory="/${scratch_directory_base}/${SLURM_JOB_ID}"
```

```
## initialize gaussian
export g16root="/sw/linux/gaussian/g16"
. ${g16root}/g16/bsd/g16.profile


printf "Hi, I am job %s on %s in %s\n" "${SLURM_JOB_ID}" "${HOSTNAME}" "${PWD}"


## Creating working directory where the job will run and produce data:
if [ ! -d "${working_directory}" ];
then
        mkdir -p "${working_directory}"
fi
## let Gaussian put temporary data into the working directory
export GAUSS_SCRDIR="${working_directory}"


## copy data to directory -- if you use checkpoint files and don't
## name them differently on purpose, copy the checkpoint file, too.
cp ${submission_directory}/${input}.com ${working_directory}
if [ -f "${submission_directory}/${input}.chk" ]; then
    cp ${submission_directory}/${input}.chk ${working_directory}
fi


printf "Starting simulation in %s\n" "${PWD}"
cd "${working_directory}"
${g16root}/g16/g16 <${input}.com >${input}.out


# copy output and checkpoint file back
cp ${input}.out ${submission_directory}
if [ -f "${input}.chk" ]; then
    cp ${input}.chk ${submission_directory}
fi

## clean up behind yourself
rm -rf "${working_directory}"
```

Listing 1: Example SLURM job script for gaussian

Gaussian 09

Gaussian 09 binaries have been installed in `/sw/linux/gaussian/g09`. To be able to use it on the thinc cluster please set the following environment variables in your Job script:.

For interactive use, if you use bash add the following lines to your `~/.profile`:

```
export g09root=/sw/linux/gaussian
ulimit -s 65536
. $g09root/g09/bsd/g09.profile

export GAUSS_SCRDIR=/usr/scratch/$LOGNAME
```

If you interactively still use legacy tcsh add those lines to your `~/.login`:

```
setenv g09root /sw/linux/gaussian
limit stacksize 65536
source $g09root/g09/bsd/g09.login

setenv GAUSS_SCRDIR /usr/scratch/$LOGNAME
```

GAUSS_SCRDIR is the scratch directory Gaussian will use.

Please make sure

- your jobscript contains the above lines for initialization (your job will probably not run in a login shell)
- that the *GAUSSDIR_SRCDIR* directory exists before calling Gaussian
- to delete all the Gaussian scratch files after your job finishes

(The Gaussian 09 Manuals are currently in the hands of Denis or members of his group)

Turbomole

Please note: to use Turbomole, your account has to be a member of the "`turbomole`" group. Please mail helpdesk ((helpdesk@mpip-mainz.mpg.de) to add you to it.

Run the following commands before using turbomole:

- Turbomole 7.3 and 6.5 (set *TURBOVERSION* to "6.5" to use version 6.5)

```
TURBOVERSION=7.3
export TURBODIR=/sw/linux/turbomole/$TURBOVERSION
. $TURBODIR/Config_turbo_env
```

- Turbomole 6.3 and 6.2 (set *COSMOVERSION* to "10" to use version 6.2)

```
COSMOVERSION=11
TURBODIR=/sw/linux/COSMOlogic${COSMOVERSION}/TURBOMOLE
PATH=$PATH:$TURBODIR/scripts
```

```
PATH=$PATH:$TURBODIR/bin/$(sysname)
export TURBODIR PATH
```